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Author(s): Remedés, Tyler Joseph
Albright, Eric Jason
Schmidt, Emma Marie
Ramsey, Scott D.

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A quick introduction to linear transport phenomena

Tyler Remedès

Jason Albright

Emma Schmidt

Scott Ramsey

Los Alamos National Laboratory

February 18, 2022

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Abstract

The goal of this report is to provide an introductory-level overview of the linear Boltzmann equation in the context of neutron transport. After deriving the transport equation, we discuss some of its basic applications in reactor theory. Finally, we review several simplifying approximations of the linearized Boltzmann equation that are essential to solving it in many applications. Although the context of neutron transport is called upon to add concreteness to our discussion, many of the concepts and approximations that we discuss remain relevant in other many other phenomena.

1 Introduction

The purpose of our document is to take someone new to the concepts of neutron transport and teach them some basics principals, hopefully in a manner that helps point them to further resources to continue their education. To this end, we begin by taking a philosophic approach to the linear Boltzmann equation, which has its roots in the kinetic theory of gases. A comprehensive reference for the Boltzmann Equation that discusses its applications to different fields and also and much more sophisticated mathematical treatment of its derivation can be found in [3]. The specific context that we will derive and discuss the linear Boltzmann equation is neutron transport. Hence, it will be helpful to start with a physical description of the neutron system that we hope to model with the transport equation. Therefore, we start with a description of the different ways neutrons interact with matter. The discussion herein is meant to orient a reader with little to no background in neutron transport and the reader may discover that some scientists and engineers take a much more nuanced approach when discussing neutron interactions.

1.1 Particle reactions

First, from the point of view of just a single, isolated neutron traveling through space the bulk part of the volume in any body of matter is *unoccupied* space. To illustrate that fact, which may sound surprising, suppose that we scaled up the radius of each nuclei of the atoms that make up the surrounding crystal lattice of matter to 30 cm, then the outermost electrons in each atom would be 30 km away (i.e., 10^5 times the size of the radius). The nearest neighboring nucleus (NNN, for short) would be another 60 km away. Even in fairly dense materials, like heavy metals, that volume of occupied space amounts to a paltry to one part in 10^{15} (ten quadrillion). And the rest? Just empty space. The actual dimensions we're talking when it comes to neutrons, nuclei, and atoms without any scaling are shown in Table 1 for reference.

Given the relatively large expanses between nuclei, together with the fact that neutrons do not carry a charge (and consequently, experience no force of attraction) you may be wondering how any interactions with surrounding matter occur at all. There are two additional factors that we haven't thought of yet, which can substantially alter the picture we have been describing so far. The first is that in most volumes of interest, e.g. a nuclear power reactor, are flooded with neutrons. Hence, the number of neutrons actually tends to be relatively large in contrast to the scenario we just described in terms of a single, isolated neutron. Second, relative to the distance between the NNN, neutrons are traveling extremely fast (8,000 to 80,000,000 km

Table 1: Physical dimensions (in round numbers) of several fundamental particles in increasing order with respect to radius. The number of protons is denoted Z and A denotes the number protons and neutrons.

Particle	Radius (cm)	Mass (g)	Charge (Coul)
Electrons	2×10^{-13}	9×10^{-28}	-2×10^{-19}
Protons	1×10^{-16}	2×10^{-24}	2×10^{-19}
Neutrons	1×10^{-16}	2×10^{-24}	0
Nuclei	1×10^{-13}	$A \cdot 2 \times 10^{-24}$	$Z \cdot 2 \times 10^{-19}$
Atoms	1×10^{-8}	$A \cdot 2 \times 10^{-24}$	0

hr^{-1}). Consequently, collisions¹ between neutrons and nuclei happen on relatively short time scales (between microseconds and milliseconds).

Now that we have some justification that we should expect a large number of very frequent collisions, let's discuss some of the different possible outcomes of individual collisions. While there are many different possible neutron interactions, we can group them all into three main categories: 1) Scattering, 2) Absorption, and 3) Fission.

Perhaps the most natural to start with is scattering. Scattering can happen in two different varieties, either elastic or inelastic. In an *elastic* collision, there is no exchange (or transfer) of kinetic energy between the two bodies, but the emitted neutron usually travels in a new direction. In contrast, in an *inelastic* collision, the incident neutron, gets caught (in a sense) in the target nucleus for just an instant before being emitted with a change in its momentum. Actually, inelastic collisions are even more complicated than this suggests, the neutron emitted by the nucleus after the collision might not be the same one that caused the collision.

The next category of interactions are *absorptions* interactions, or in this sense “capture” interactions. Depending on the energy level of the incident neutron (and perhaps the direction it is traveling), the neutron could just be absorbed by the target nucleus without escaping, consequently leaving the target nucleus in an excited energy state (think of a raindrop alternating between stretching and contracting in multiple directions). After the absorption, there are several ways for the excited nucleus to de-excite. There are many ways an excited nucleus could de-excite, some of these are: the emission of light as a gamma ray, the emission of multiple neutrons (conservation of momentum still applies here however!), and the emission of a charged particle (i.e.; protons, alpha particles, electrons).

Finally, if the incident neutron is moving rapidly enough, it could smash into the nucleus with enough force to break it into fragments (in analogy to the raindrop, enough tension caused by the stretching and contracting would cause it to break apart into smaller droplets) causing a *fission* reaction. In a sense fission is a type of absorption interaction since the incoming neutron is absorbed before the nucleus breaks apart. To this end, you may hear people consider fission as a type of absorption reaction in day-to-day conversations and they would be right to do so (something to note, typically if a person says “capture” reaction they are referring to absorption type reactions without fission. And if a person says “absorption” reaction, they mean capture + fission.). However, we wanted to break fission reactions apart from absorption reactions (no pun intended) because fission events are handled specially in the Boltzmann transport equation. Its most important feature is that, in addition to breaking apart the incident nucleus, it is accompanied by the emission of more than one neutron. Although, we have over simplified all three types of reactions described here, the general picture is that all neutron-nuclei reactions can be placed into one of three categories as we have defined them: scattering, absorption, and fission, and all three reactions have a different net effect on the redistribution of our population following a collision.

You may have noticed that that the preceding list of interactions did not include collisions between neutrons with themselves. You might be wondering, why not? Although, we have assumed that the region of interest contains a large number of neutrons (in the sense that interactions with the surrounding nuclei occur on relatively short time scale relative to the distance separating them), the number of nuclei relative to the number of neutrons is relatively much larger. This, in addition to the fact that the range of interaction forces between neutrons is also several orders of magnitude smaller than the range of influence of intermolecular forces, neutron-neutron collisions are likely infrequent enough that they will be neglected (See Lewis and Miller [9] and Cercignani [3] for further justification). Mathematically, leaving out neutron-neutron, or more generically particle-particle interactions, has a number of important

¹Carrying on with the suggestion that neutrons undergo gentle *interactions* with matter would be a supreme understatement taking into account that even the more modest of these incidents that involve particles screaming through space at $8,000 \text{ km hr}^{-1}$ is closer to an astroid impact with a planet...relatively speaking, of course.

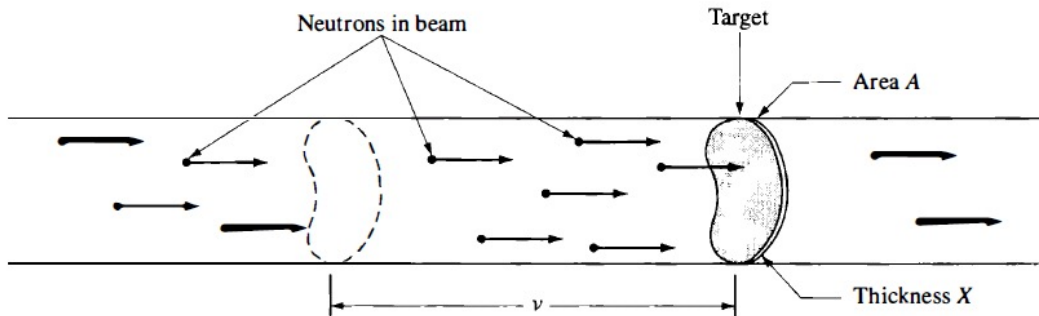


Figure 1: A beam of neutrons is traveling through a target.

consequences, although we will not formally demonstrate it explicitly as part of our derivation of the transport equation in Section 3. In general, the Boltzmann equation is reduced to the linear Boltzmann equation by assuming particle-particle interactions do not occur. This distinguishes neutron transport from other, perhaps more familiar types of transport processes, like classical statistical mechanics. In statistical mechanics we are concerned with particles interacting with themselves, which is the main source of nonlinearity in the forms of the Boltzmann equations that describe these processes. It is worth having this important assumption (the assumption that we can neglect neutron-neutron interactions) in mind since it will play an underlying role in informing how we can solve the neutron transport equation in Sections 4 and 5.

1.2 Nuclear cross sections

Given the complexity of the interactions between an incident neutron and a target nucleus, it is not feasible (at this point in time given that this is likely a wholly intractable set of quantum mechanical calculations featuring nuclei with highly complicated energy structure) to predict with any degree of certainty the particular mechanism through which the nucleus will de-excite following a collision, e.g., neutron re-emission via inelastic scattering or gamma ray emission via absorption. However, given a suitably large population and a sufficient number of interactions, we can measure the relative frequency of each type of interaction, which then allows us to formulate probabilistic-type predictions regarding outcomes of isolated interactions. Estimating these probabilities requires conducting actual experiments. Moreover, from our simplified description of nuclear reactions above, we know that these statistics we could collect are dependent on the (kinetic) energy of the incident neutron and the species of nuclei that the neutrons are interacting with.

This probabilistic aspect of the model is encapsulated in the notion of a nuclear cross section, invented for this exact purpose by ingenious physicists. To introduce the idea of a nuclear cross section, consider a volume of space in the shape similar to a cylinder, shown in Fig. 1, with length Δu and cross sectional area ΔA occupied by a concentration of n atoms/cm³. Next, suppose we direct a beam emitting one neutron at a time traveling in the direction normal to one end of our cylinder and that the thickness of the cylinder Δu is sufficiently small to guarantee that the atoms occupying the cylinder do not overlap one another (i.e., our cylinder is probably proportioned more like a quarter than a can of soup). If we observe enough neutrons, the probability of a collision with one of the atoms occupying the cylinder is equivalent to the ratio of the cross sectional area “shadowed” by the occupying atoms to the cross sectional area of the unoccupied space. If we denote the cross sectional area of each atom as A_a , then this ratio is

$$p = \frac{A_a n \Delta V}{\Delta A} = \frac{A_a n \Delta A \Delta u}{\Delta A} = n A_a \Delta u. \quad (1)$$

In the context of the experiment, the probability p is the observable (measurable), and the

nuclear cross section A_a is treated as unknown. Hence, after we have collected enough data to be confident in our value for p , we can use Equation (1) to solve for A_a , which is called the *microscopic cross section*².

Now, here's the take away from this Gedank of sorts. We usually aren't too interested in the microscopic cross section of an atomic species. Instead, we are interested in a related quantity called the *macroscopic cross section* denoted σ . The *macroscopic cross section* is the product of the microscopic cross section and the concentration of atoms n , i.e.,

$$\sigma = nA_a. \quad (2)$$

Since σ will turn out to be an important quantity that we will need later, let's examine its units. Notice that in terms of the probability p from Equation (1),

$$\sigma = \frac{p}{\Delta u}, \quad (3)$$

Recall, that Δu was chosen to guarantee that no atoms are overlapping in our cylinder, if Δu is also exactly a path length (the average distance between collisions) than we would expect at most one interaction per neutron in our cylinder in unit time. Therefore, the the macroscopic cross section³ σ is just

$$\sigma = \text{probability of an interaction per unit path length during } \Delta t, \quad (4)$$

where Δt is the transit time of a neutron (at a fixed energy) through the cylinder.

Recall that the energy of the neutrons affects the likelihood of certain reactions, hence we need to repeat this experiment for different neutron energies E . Next, if we keep track of the nuclear species occupying a given region of space according to their position by \mathbf{x} , then the total macroscopic cross section is a function of the form $\sigma = \sigma(\mathbf{x}, E)$.

It is also helpful to break up the total macroscopic cross section into the contributions from different reactions. For a reaction of type x , the corresponding macroscopic cross section is denoted σ_x . Therefore, the total macroscopic cross section σ is the sum of all partial cross sections σ_x for all possible types of neutron-nucleus collisions,

$$\sigma(\mathbf{x}, E) = \sum_x \sigma_x(\mathbf{x}, E). \quad (5)$$

For example, if we want to know that total probability (per unit path length) of a reaction assuming just scattering and fission, then

$$\sigma = \sigma_s + \sigma_f, \quad (6)$$

where the subscripts s and f denote elastic scattering and fission, respectively.

1.3 Further reading

There are two texts in particular which we believe provide a lengthier discussion of the topics provided in this section at an introductory level. The first is *Fundamentals of Nuclear Reactor Physics* by E. E. Lewis [8]. Lewis provides great discussion of basic concepts (such as cross sections, mean free paths, and reaction types) using a very fundamental approach. We believe his physics-based approach to the topic complements our geometry-based discussion provided in

²The units of microscopic cross sectional area are measured in cm^2 , however, it is customary to use the units of barns, equivalent to 10^{-24}cm^2 . Why you ask? Because even the broadside of a barn is not so easy to hit under the assumption of negligible atomic cross sectional area.

³Most texts use Σ to denote the macroscopic cross section and σ to denote the microscopic cross section. As it turns out, this notation creates a conflict with the use of Σ for sums. Since we will mainly deal with the macroscopic cross section, we will use σ throughout.

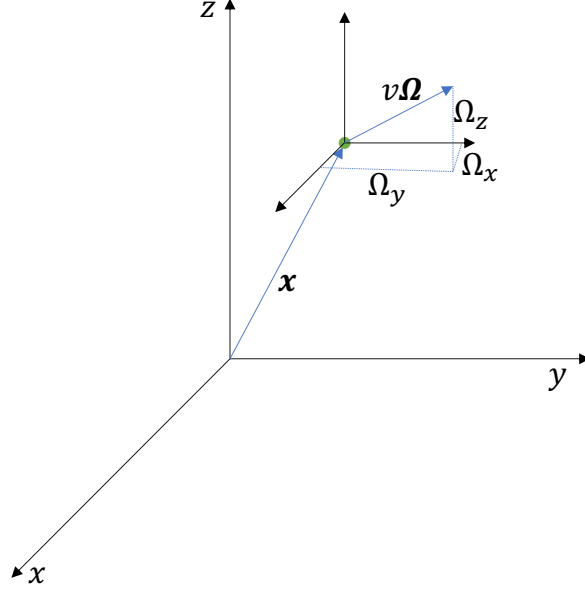


Figure 2: The neutron is positioned at location \mathbf{x} and is traveling with a velocity given by $v\mathbf{\Omega}$. Note that the location vector of the neutron and the direction vector of the neutron are two separate quantities.

the previous section. Lamarsh and Baratta's [7] work titled *Introduction to Nuclear Engineering* is another great work providing an easy to follow introduction to nuclear engineering concepts. Lamarsh and Baratta, however, is considered by some as a more complicated text than Lewis. That being said, Lamarsh and Baratta remains an excellent resource for those new to nuclear engineering. Some readers may find it helpful to begin with Lamarsh and Baratta and use Lewis to explain some of the more complex ideas in Lamarsh and Baratta. On a final note, both these resources use a slightly different notation than what is used in this document. We choose a notation commonly used in more advanced nuclear engineering texts. Our hope is to educate a novice reader to a point where they could reference these advanced texts. It is our hope that the differences in notation do not discourage any readers, rather that demonstrates the various notational styles of nuclear scientists and engineers.

2 Notation

Before starting our derivation of the equation, we need to introduce some useful notation that will be called upon later.

Figure 2 shows the position of a neutron is given by a vector \mathbf{x} (in three space $\mathbf{x} = (x, y, z)$). The velocity \mathbf{v} of a neutron is given by⁴

$$\mathbf{v} = v\mathbf{\Omega}, \quad (7)$$

where $v = |\mathbf{v}|$ is the speed of neutron and $\mathbf{\Omega} = (\Omega_x, \Omega_y, \Omega_z)$ is a unit vector describing the direction of the neutron's velocity. One thing to note it that v , or rather E^5 , and $\mathbf{\Omega}$ can take any value within the continuous range of $0-\infty$ and $0-4\pi$ respectively. In three space, the direction is given by

$$\Omega_x = \sin \theta \cos \varphi, \quad \Omega_y = \sin \theta \sin \varphi, \quad \Omega_z = \cos \theta, \quad (8)$$

⁴It is important to note that this velocity quantity is the velocity of individual neutrons and is more akin to a particle velocity rather than to a mean field velocity which is averaged over a number of elements.

⁵The neutron's kinetic energy given by $E = 1/2m_nv^2$ with m_n being the neutron mass.

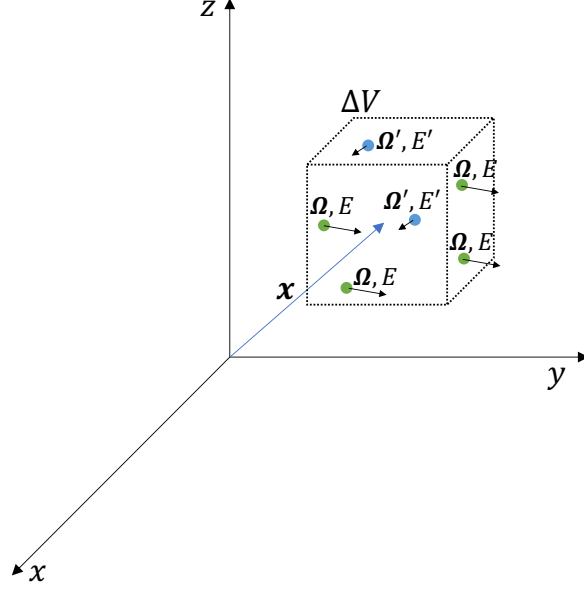


Figure 3: A group of neutrons exists in ΔV . Each neutron is labeled with its direction and energy values and are color coded by the packet in which they belong. Even though both the green and blue neutrons are in the same ΔV , they have different energies and are traveling in different directions. The result is that the green neutrons form one packet and the blue neutrons form another packet.

where θ and φ denote the polar and azimuthal angles, respectively.

The kinetic energy of a neutron is determined from its velocity according to

$$E = \frac{mv^2}{2}, \quad (9)$$

where m denotes the mass of a neutron. Hence, given a neutron's position \mathbf{x} , we must also characterize it in terms of its direction of flight $\boldsymbol{\Omega}$ and its kinetic energy E .

2.1 Number density and flux

To track larger populations of neutrons in a given region of space, it is useful to introduce a quantity called the *angular (number) density*, denoted

$$\text{Angular (number) density} = N(\mathbf{x}, \boldsymbol{\Omega}, E, t). \quad (10)$$

The *angular density* is defined as the expected number of particles at \mathbf{x} traveling in the direction $\boldsymbol{\Omega}$ with energy E at time t per unit volume per unit solid angle per unit energy. All these trailing “pers” are simply a helpful reminder that

$$\begin{aligned} N(\mathbf{x}, \boldsymbol{\Omega}, E, t) \Delta V \Delta \Omega \Delta E &= \text{the expected number of neutrons at } \mathbf{x} \\ &\text{traveling along } \boldsymbol{\Omega} \text{ with energy } E \text{ at time } t, \\ &\text{in volume } \Delta V \text{ within } \Delta \Omega \text{ and } \Delta E. \end{aligned} \quad (11)$$

It is also helpful to further interpret this notation as categorizing the population of neutrons in a volume ΔV into *packets* or *groups* of neutrons with two labels, shown in Fig. 3. The green neutrons form one packet in ΔV as these neutrons share a common direction and energy values $(\boldsymbol{\Omega}, E)$ and the blue neutrons form a second packet - since they have similar direction and

energy values with each other (Ω', E') but different than the green neutrons. The first “label” indicates its direction of flight in terms of a specific cone of directions $\Delta\Omega$ oriented along Ω and the second label indicates the neutron’s energy defined in terms of an interval ΔE about E . Over time we are interested in the change in the population of each packet defined by a pair of labels. As a preview of one of the topics we will get to later, is that in practice it is possible to choose a manageable (finite) number of discrete angles and energies (or equivalently velocities) to approximate their corresponding continuous spectra.

Our goal will be to eventually solve for the neutron flux. The neutron flux is important as this quantity describes the neutron population distribution. Moreover, understanding how neutrons are distributed in a system is foundational to determining other quantities of interest such as how much radiation dose a person has received, how well will a nuclear reactor produce power, can we use radiation to image the inside of a hospital patient, and other such questions. However, there are still several other important quantities related to the angular density which we need to define before we can turn our attention to the neutron *flux*. The product of the velocity and the angular density gives an important quantity called the *vector flux*

$$\text{Vector flux} = \mathbf{v}N(\mathbf{x}, \Omega, E, t). \quad (12)$$

Integrating the vector flux over all incident directions gives the *neutron current density* denoted $\mathbf{J}(\mathbf{x}, E, t)$, i.e.,

$$\mathbf{J}(\mathbf{x}, E, t) = \int_{4\pi} \mathbf{v}N(\mathbf{x}, \Omega, E, t) d\Omega. \quad (13)$$

The neutron current isn’t exactly the most used quantity in nuclear engineering. Rather, nuclear engineers tend to care about the total flux. To find the total flux, we first take the magnitude of vector flux in Equation (12) in order to find the *angular flux*,

$$\text{Angular flux} = vN(\mathbf{x}, \Omega, E, t) = \psi(\mathbf{x}, \Omega, E, t). \quad (14)$$

Then the *total flux*, that is the number of neutrons at \mathbf{x} with energy E at time t , is given by

$$\text{Total flux} = \int_{4\pi} \psi(\mathbf{x}, \Omega, E, t) d\Omega. \quad (15)$$

Usually, the total flux is denoted $\phi(\mathbf{x}, E, t)$. The total flux is usually the quantity we are solving for in our problems. Fluxes are generated by sources, which we will separate into external sources and internal sources. We consider internal sources as neutron transfer and multiplication and these concepts will be handled subsequently. However, we will conduct our discussion of external neutron sources now.

2.2 Transfer probabilities

In this section, we return to the *macroscopic cross section* of a neutron introduced earlier. Recall,

$$\sigma = \text{probability per unit path length of a collision in } \Delta t. \quad (16)$$

The macroscopic cross section has units $length^{-1}$ and is usually taken as a function $\sigma(\mathbf{x}, E)$. The remaining piece that must be built into the macroscopic cross section is that neutrons emitted after a collision will assume a distribution of different directions of emission and energies. Herein lies the reason transfer probabilities are considered source terms, since these complicated expressions describe how neutrons move from one packet into another. Since these outcomes cannot be predicted for individual collisions, we again turn to probability to model this feature.

For a reaction of type x , the probability that particles traveling with initial direction Ω' and initial energy E' are emitted traveling in direction Ω with energy E after the reaction is defined in terms of the

$$\text{Differential cross section} = \sigma_x(\mathbf{x}, E') f_x(\mathbf{x}, \Omega' \rightarrow \Omega, E' \rightarrow E). \quad (17)$$

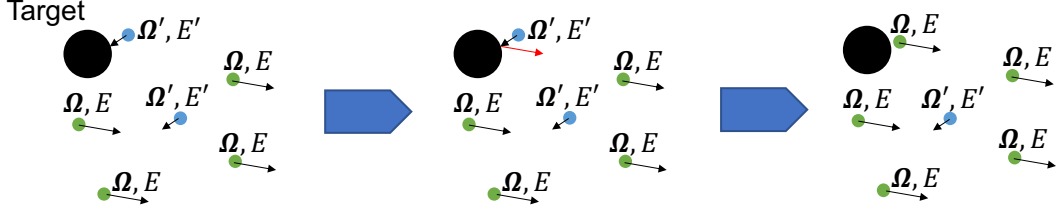


Figure 4: Here we show how a scattering interaction moves a neutron from one packet into another. In the leftmost image, a blue neutron undergoes a scattering interaction with a target nucleus. The second image shows the neutron's change in energy and direction with a red arrow and the third image shows the neutron now traveling in the same packet as the green neutrons.

The quantity $f_x(\mathbf{x}, \Omega' \rightarrow \Omega, E' \rightarrow E) \Delta\Omega \Delta E$ is the probability that a particle traveling with initial direction Ω' and initial energy E' is emitted traveling in direction Ω in the cone of directions $\Delta\Omega$ with energy E in the interval ΔE after the reaction. The two interactions that provide a source of neutrons which we are most concerned with are scattering and fission⁶. Again, the function f_x must be obtained from approximations to data for each nuclear species and reaction type present in the domain of interest. With the exception of fission reactions, which we treat subsequently immediately below, the differential cross sections are usually treated as normalized so that

$$\int \int_{4\pi} f_x(\mathbf{x}, \Omega' \rightarrow \Omega, E' \rightarrow E) d\Omega dE = 1. \quad (18)$$

In what follows, we will frequently write $\sigma' f' = \sigma(\mathbf{x}, E') f(\Omega' \rightarrow \Omega, E' \rightarrow E)$ to reduce notation.

Figure 4 shows the process by which a neutron scatters from one energy group to another. In this image, a neutron is traveling with direction Ω' with energy E' and scatters off a target nucleus. In this context, a target nucleus is simply a nucleus belonging to the bulk matter that the neutrons are traveling through. The scatter interaction causes a change in the neutron's direction and energy, shown by the red arrow in the second picture of Fig. 4. After the interaction, the neutron is now traveling in direction Ω with energy E , denoted by the change in color of our neutron. If we assume that the neutrons are emitted uniformly in all directions (isotropically), then for scattering reactions system, the differential cross section has the form

$$f_s(\mathbf{x}, E' \rightarrow E) = \frac{1}{4\pi}, \quad (19)$$

since all angles are equally possible under the isotropic scattering assumption.

Another interaction that acts as a neutron source is fission. In the case of fission, a neutron interacts with a target nucleus shown in the first image in Fig. 5, and causes a fission event denoted by the star in the second image. Neutrons are released as a result of fission (two neutrons in our example), and one of these neutrons happens to be traveling in direction Ω with energy E . For the case of fission reactions we assume that the neutrons are emitted isotropically, then the differential cross section for fission is usually re-expressed in terms of

$$f_f(\mathbf{x}, \Omega' \rightarrow \Omega, E' \rightarrow E) \Delta\Omega \Delta E = \frac{1}{4\pi} \nu(E') f(\mathbf{x}, E' \rightarrow E) \Delta\Omega \Delta E. \quad (20)$$

⁶It may not be readily apparent how scattering acts as a neutron source. Recall how we have considered our neutron packets as groups of neutrons traveling with similar energies and in similar directions. Scattering acts as a neutron source because a neutron from one packet (with energy E' and direction Ω') can undergo a scattering interaction and then have energy E and direction Ω , therefore adding a neutron to our group. You may wonder how we account for this neutron being lost from its original packet. This is accounted for in the total cross section which determines the number of neutrons lost from a packet by all forms of interactions.

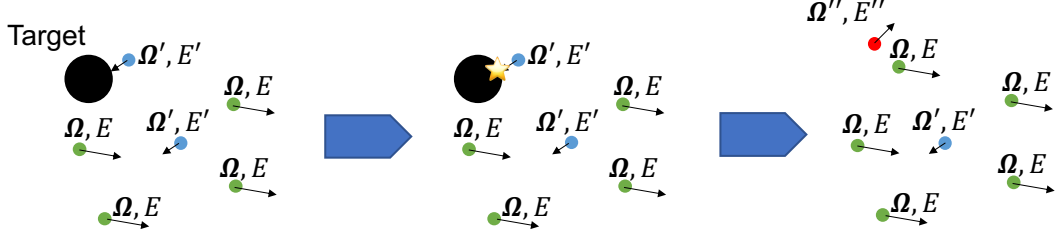


Figure 5: Another interaction that acts a neutron source is fission. In the first image, a neutron interacts with a target nucleus and causes a fission event, denoted with the star in the second image. The fission event causes two neutrons to be born with different energy values and traveling in different directions. One of those neutron is traveling in direction Ω with energy E .

The quantity $\nu(E)$ is the expected number of neutrons emitted in a fission with an incident neutron with energy E' . The distribution $f(\mathbf{x}, E' \rightarrow E)\Delta E$ is called the *fission spectrum of neutrons*, and is usually denoted $\chi(E)$ ⁷ (see [9] for more details). In several subsequent sections, to emphasize the assumption of isotropic emission, we will also use $\chi(E)$ in order to distinguish this distribution from the more differential cross section $f_f(\mathbf{x}, \Omega' \rightarrow \Omega, E' \rightarrow E)$. The fission spectrum quantifies the probability that an incident neutron with energy E' will lead to a neutron emitted with energy ΔE about E . Usually, $\nu(\mathbf{x}, E' \rightarrow E)$ is expressed in terms of an average $\bar{\nu}$ determined by

$$\bar{\nu} = \frac{1}{4\pi} \int \int_{4\pi} \nu(\mathbf{x}, E' \rightarrow E) \chi(\mathbf{x}, E' \rightarrow E) d\Omega dE = \int \nu' \chi' dE. \quad (21)$$

The integral $\bar{\nu}$ is the average number of neutrons produced by a fission at \mathbf{x} by an incident neutron with energy E' .

However, in general (without the assumption of isotropic emission), we will assume f is normalized so that

$$\int \int_{4\pi} f(\mathbf{x}, \Omega' \rightarrow \Omega, E' \rightarrow E) d\Omega' dE' = \sum_x c_x \sigma_x(\mathbf{x}, E) = c(\mathbf{x}, E). \quad (22)$$

Hence, for example

$$c(\mathbf{x}, E) = \frac{\sigma_s(\mathbf{x}, E) + \bar{\nu} \sigma_f(\mathbf{x}, E) + \dots}{\sigma(\mathbf{x}, E)}, \quad (23)$$

where $c_s = 1$ for elastic scattering and $c_f(\mathbf{x}, E) = \bar{\nu} c(\mathbf{x}, E)$ for fission.

Finally, we arrive at the concept of a *transfer probability*, which describes the probability of neutron transferring from one angle-energy packet to another after a collision. Since $\sigma(\mathbf{x}, E)$ is the total cross section,

$$\begin{aligned} \text{Total probability of neutron transfer} &= \sigma(\mathbf{x}, E') f(\mathbf{x}, \Omega' \rightarrow \Omega, E' \rightarrow E), \\ \text{from } \Omega' \text{ to } \Omega \text{ and } E' \text{ to } E & \end{aligned} \quad (24)$$

where

$$\sigma(\mathbf{x}, E') f(\mathbf{x}, \Omega' \rightarrow \Omega, E' \rightarrow E) = \sum_x \sigma_x(\mathbf{x}, E') f_x(\mathbf{x}, \Omega' \rightarrow \Omega, E' \rightarrow E). \quad (25)$$

Now we can quantify the total rate at which particles are transferred from one packet to another after reaction x in terms of the transfer probability. At time t and position \mathbf{x} , the reaction rate

⁷We typically use the Watt fission spectrum to describe $\chi(E)$.

in neutrons per volume is given by

$$\begin{aligned} \text{Total reaction rate from } \boldsymbol{\Omega}' \text{ to } \boldsymbol{\Omega} \text{ and } E' \text{ to } E &= v(E')\sigma_x(\mathbf{x}, E')f_x(\mathbf{x}, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}, E' \rightarrow E) \\ &\cdot N(\mathbf{x}, \boldsymbol{\Omega}, E, t)\Delta V\Delta\boldsymbol{\Omega}\Delta E. \end{aligned} \quad (26)$$

In particular, by multiplying the differential cross section by the velocity of the incident neutron v_x , the units on the right hand side reactions per unit time. Therefore, the total rate at which neutrons are transferred can be obtained by integrating expression (26) over all angles and all energies, and summing over all reactions (indexed by x)

$$\int \int_{4\pi} v(E')\sigma(\mathbf{x}, E')f(\mathbf{x}, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}, E' \rightarrow E)N(\mathbf{x}, \boldsymbol{\Omega}, E, t)d\boldsymbol{\Omega}dE\Delta V. \quad (27)$$

3 Derivation

In this section, we will derive the neutron transport equation as a balance law for the neutron population that accounts for both the gains and the losses due to the three fundamental processes of collision, streaming, and source production described in previous sections. The treatment of the basic derivation follows closely the presentation in [1].

Recall, the quantity $N(\mathbf{x}, \boldsymbol{\Omega}, E, t)\Delta V\Delta\boldsymbol{\Omega}\Delta E$ is the expected number of neutrons in volume ΔV centered at \mathbf{x} , traveling within the cone of directions $\Delta\boldsymbol{\Omega}$ centered around direction $\boldsymbol{\Omega}$, with energy ΔE about E at time t that is shown in Fig. 3. To derive the neutron transport equation, we will consider the probable changes to this group or packet of neutrons over a time interval Δt .

First, the neutrons with energy E that are involved in a collision in ΔV will be considered lost from the packet, and those that do not collide will continue to stream within $\Delta\boldsymbol{\Omega}$ about $\boldsymbol{\Omega}$. Since the number of path lengths traveled in Δt is $v\Delta t$ and the probability per unit path length of a collision is $\sigma(\mathbf{x}, E)$, the probability per unit path length of that the packet undergoes zero collisions is $1 - \sigma(\mathbf{x}, E)$. Therefore, the number of neutrons remaining in the packet is

$$\begin{aligned} \text{Number of neutrons} &= N(\mathbf{x}, \boldsymbol{\Omega}, E, t)[1 - \sigma(\mathbf{x}, E)v\Delta t]\Delta V\Delta\boldsymbol{\Omega}\Delta E. \\ \text{remaining in packet} & \end{aligned} \quad (28)$$

Since the packet is traveling in direction $\boldsymbol{\Omega}$, the remaining neutrons in the packet will arrive at $\mathbf{x} + v\Delta t\boldsymbol{\Omega}$ after Δt .

Next, the number of neutrons in the packet can also increase as a result of collisions that cause neutrons from outside the packet to transfer into the packet. Recalling that the differential cross section $\sigma_x f_x$ is the probability per unit length that after a reaction of type x a neutron traveling initially in direction $\boldsymbol{\Omega}'$ with energy E' will emerge traveling within the cone $\Delta\boldsymbol{\Omega}$ about $\boldsymbol{\Omega}$ and in the interval ΔE about energy E , the expected number of neutrons joining the packet is given by

$$\int \int_{4\pi} v'\sigma(\mathbf{x}, E')f(\boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}, E' \rightarrow E)N(\mathbf{x}, \boldsymbol{\Omega}, E, t)d\boldsymbol{\Omega}'dE'\Delta V\Delta\boldsymbol{\Omega}\Delta E\Delta t. \quad (29)$$

Finally, neutrons can also be added from external sources. The source rate is denoted $q(\mathbf{x}, \boldsymbol{\Omega}, E, t)$, and so the contribution to the packet from external sources is

$$\begin{aligned} \text{Number of neutrons entering} &= q(\mathbf{x}, \boldsymbol{\Omega}, R, t)\Delta V\Delta\boldsymbol{\Omega}\Delta E\Delta t. \\ \text{from external sources} & \end{aligned} \quad (30)$$

Therefore, tallying the number of neutrons in the packet after Δt by adding all three terms together (and dividing by $\Delta V \Delta \Omega \Delta E$) yields,

$$\begin{aligned} N(\mathbf{x} + v\Delta t \mathbf{\Omega}, \mathbf{\Omega}, E, t + \Delta t) = & N(\mathbf{x}, \mathbf{\Omega}, E, t)[1 - v\Delta t \sigma(\mathbf{x}, E)] \\ & + \int \int_{4\pi} v' \sigma' f' N(\mathbf{x}, \mathbf{\Omega}, E, t) d\mathbf{\Omega}' dE' \Delta t \\ & + q(\mathbf{x}, \mathbf{\Omega}, E, t) \Delta t \end{aligned} \quad (31)$$

Next, after rearranging and dividing by Δt we obtain

$$\begin{aligned} \frac{N(\mathbf{x} + v\Delta t \mathbf{\Omega}, \mathbf{\Omega}, E, t + \Delta t) - N(\mathbf{x}, \mathbf{\Omega}, E, t)}{\Delta t} = & v\sigma N(\mathbf{x}, \mathbf{\Omega}, E, t) \\ & + \int \int_{4\pi} v' \sigma' f' N(\mathbf{x}, \mathbf{\Omega}, E, t) d\mathbf{\Omega}' dE' \\ & + q(\mathbf{x}, \mathbf{\Omega}, E, t) \end{aligned} \quad (32)$$

In order to compute the limiting value as $\Delta t \rightarrow 0$ on the left hand side, as an intermediate step we need to subtract and then add $N(\mathbf{x}, \mathbf{\Omega}, E, t + \Delta t)$ back in. The limit of the original difference quotient in the previous equation can then be split into two terms

$$\begin{aligned} \lim_{\Delta t \rightarrow 0} \frac{N(\mathbf{x} + v\Delta t \mathbf{\Omega}, \mathbf{\Omega}, E, t + \Delta t) - N(\mathbf{x}, \mathbf{\Omega}, E, t + \Delta t)}{\Delta t} \\ + \lim_{\Delta t \rightarrow 0} \frac{N(\mathbf{x}, \mathbf{\Omega}, E, t + \Delta t) - N(\mathbf{x}, \mathbf{\Omega}, E, t)}{\Delta t}. \end{aligned} \quad (33)$$

From which we recognize, the second term is just a partial derivative with respect to time

$$\frac{\partial N}{\partial t} = \lim_{\Delta t \rightarrow 0} \frac{N(\mathbf{x}, \mathbf{\Omega}, E, t + \Delta t) - N(\mathbf{x}, \mathbf{\Omega}, E, t)}{\Delta t}, \quad (34)$$

and the second term is the directional derivative

$$v\mathbf{\Omega} \cdot \nabla N = \lim_{\Delta t \rightarrow 0} \frac{N(\mathbf{x} + v\Delta t \mathbf{\Omega}, \mathbf{\Omega}, E, t + \Delta t) - N(\mathbf{x}, \mathbf{\Omega}, E, t + \Delta t)}{\Delta t}. \quad (35)$$

This may be a good opportunity for you to dust off your favorite calculus textbook, such as [6].

Summing up, we obtain the *time-dependent neutron transport equation*

$$\frac{\partial N}{\partial t} + v\mathbf{\Omega} \cdot \nabla N + \sigma v N = \int \int_{4\pi} v' \sigma' f' N' d\mathbf{\Omega}' dE' + q(\mathbf{x}, \mathbf{\Omega}, E, t). \quad (36)$$

Recalling that $\psi = vN$, we can also write the neutron transport equation in the form

$$\frac{1}{v} \frac{\partial \psi}{\partial t} + \mathbf{\Omega} \cdot \nabla \psi + \sigma \psi = \int \int_{4\pi} \sigma' f' \psi' d\mathbf{\Omega}' dE' + q(\mathbf{x}, \mathbf{\Omega}, E, t). \quad (37)$$

We can further expand the reaction term on the right hand side of the equation, in this case according to contributions from scattering and fission, recall what we did in Sec. 2.2.

$$\begin{aligned} \frac{1}{v} \frac{\partial \psi}{\partial t} + \mathbf{\Omega} \cdot \nabla \psi + \sigma(\mathbf{x}, E) \psi = & \int \int_{4\pi} \sigma f' \psi' d\mathbf{\Omega}' dE' + q(\mathbf{x}, \mathbf{\Omega}, E, t) \\ = & \int \int_{4\pi} (\sigma_s f'_s + \nu \sigma_f \chi) \psi' d\mathbf{\Omega}' dE' + q(\mathbf{x}, \mathbf{\Omega}, E, t) \\ = & \int \int_{4\pi} \sigma_s f'_s \psi' d\mathbf{\Omega}' dE' + \int \nu \sigma_f \chi \int_{4\pi} \psi' d\mathbf{\Omega}' dE' + q(\mathbf{x}, \mathbf{\Omega}, E, t). \end{aligned} \quad (38)$$

The second term of the right hand side represents the neutrons produced from fission. It can also be expanded further into the form

$$\int \sigma_f \nu(E') \chi(E) \int_{4\pi} \psi' d\Omega' dE' = \chi(E) \int \nu(E') \sigma_f \int_{4\pi} \psi' d\Omega' dE' \quad (39)$$

Replacing these terms in the previous equation, the transport equation can be written

$$\frac{1}{v} \frac{\partial \psi}{\partial t} + \mathbf{\Omega} \cdot \nabla \psi + \sigma(\mathbf{x}, E) \psi = \int \int_{4\pi} \sigma_s f'_s \psi' d\Omega' dE' + \chi(E) \int \nu' \sigma'_f \int_{4\pi} \psi' d\Omega' dE' + q(\mathbf{x}, \mathbf{\Omega}, E, t), \quad (40)$$

where we have finally arrived at the full expression for the time-dependent neutron transport equation including fission and an external source.

3.1 External neutron sources

So far we have only discussed the neutron source term q as a general nebulous concept. That is in part because the external source term is handled on a case-by-case basis. Our intensions here is to provide you with enough information that you could make an external neutron source term on your own.

We would like to begin our discussion with a brief dimensional analysis. We know the neutron transport equation describes the number of neutrons in a volume at a point in time. In essence, this means the units must be $\frac{\text{neutrons}}{\text{Length}^3 \text{Time}}$, or in SI units $\frac{\text{neutrons}}{\text{cm}^3 \text{s}}$. We can check out intuition by looking at one term in the neutron transport equation. Let's look at the third term from Eqn. 40:

$$\sigma \psi = [\text{cm}^{-1}][\text{neutrons cm}^{-2} \text{s}^{-1}] = [\text{neutrons cm}^{-3} \text{s}^{-1}]. \quad (41)$$

So that checks out. Remember these units when you are asked to make a source term for yourself! Case and Zweifel's[2] book titled *Linear Transport Theory* provides the most detailed explanation of neutron sources describing detailed mathematical description of planar, spherical shell and cylindrical shell source geometries. However, the mathematical explanations used may intimidate some readers. Lamarsh and Baratta[7] provide a more understandable, yet limited, explanation of sources in simplified geometries in *Introduction to Nuclear Engineering*. Duderstadt and Hamilton's[4] book *Nuclear Reactor Analysis* sits between the two previously mentioned books in terms of mathematical rigor and number of examples.

For our discussion, we will categorize neutron sources into two types:

1. flux-driven sources (sometimes called "irradiation") and,
2. decay reactions.

The distinction is made by how the source strength, or the number of neutrons per volume per unit time, varies with the radiation flux. In flux-driven sources, the source strength changes proportionally with the radiation flux. That is because these sources produce neutrons through reactions that occur when radiation interacts with matter. Decay reaction sources do not depend on a radiation flux. Instead, these decay reactions, or simply decays, occur when a nucleus is left in an unstable energy state and release neutrons to relax to a more energetically stable state. We will now provide a brief description of each type of source as well as some examples.

Flux-driven sources

Fission is perhaps the most well known of the flux-driven sources. Certain nuclei will absorb an incoming neutron, but the energy from the extra neutron causes the nucleus to become unstable and violently break apart into two new nuclei (daughter products) and emit two or

more neutrons. While fission is likely the most well-known flux-driven neutron source, there are many more. Typically, flux-driven neutron sources are written in the form $A(X, Yn)B$. This is a condensed way to express a neutron producing nuclear reaction. The incoming particle, X , hits the target nucleus, A , and produces a number of neutrons, where Y is an integer number, and product nucleus B . In the case of fission, B is the product of two nuclei, since there are two daughter products. Some common examples of neutron sources are:

1. $A(\alpha, n)B$,
2. $A(n, Yn)B$ (i.e. $(n, 2n)$, $(n, 3n)$),
3. $A(\gamma, n)B$.

The first item in the list is called an “alpha n” reaction since an α particle (a particle made of two neutrons and two protons) is absorbed by the target nuclei and a neutron is produced by the reaction. The second item describes reactions where a neutron is absorbed by a nucleus and multiple neutrons are ejected by the unstable nucleus. The final item on the list occurs when a gamma ray with sufficient energy is absorbed by a nucleus and a neutron is emitted. The previous list is not exhaustive, rather it is our intention to provide a few examples and short descriptions in order to introduce the reader to flux-driven neutron sources.

As the name suggests, flux-driven sources depend on the flux. In fact, making a flux-driven source actually looks like a reaction rate⁸ where you say

$$q = \frac{\text{Probability of Reaction } x \text{ occurring}}{\text{Reaction } x \text{ occurring}} = \psi \sigma_x. \quad (42)$$

Equation 42 tells us how frequently, or how probable, the reaction x occurs. Then, a flux-driven source can be made by substituting σ_x for the cross section value that produces neutrons.

Decay reaction sources

Decay reaction sources, or more simply “decay reactions/sources” or “decays”, are a type of neutron source where a nucleus initially is in an energetically unstable state and relaxes to a more stable state by giving off neutrons. Spontaneous fission and delayed neutron sources are two common sources of decay reaction neutron sources. Spontaneous fission occurs naturally in some isotopes. When certain nuclei are energetically unstable, they will fission in order to get rid of excess energy. Spontaneous fission events create two daughter products and release neutrons, similar to flux-driven fission.

Delayed neutrons are a special type of neutron emission that occurs in daughter products after a fission or spontaneous fission event. Daughter products are often left in energetically unstable configurations and need to release energy in order to relax to a more energetically favorable state. Sometimes, neutrons are emitted as the daughter products relax. However, since these neutrons are emitted within milliseconds after the original fission event, they are called “delayed neutrons.”

Making a decay source term is mathematically fairly straightforward as it only depends on the activity of the neutron producing isotope, or more specifically, the decay rate of the isotope, α . The units of α are [*decays s*⁻¹], which means we need to account for the number of neutron per decay, N_n , and the volume of the isotope, V_i . Using this information leads to the expression

$$q = \alpha * N_n * V_i. \quad (43)$$

⁸Reaction rates are another common quantity in nuclear engineering because they tell us how often a certain reaction happens. The type of reaction rate is determined by the cross section used in Eqn. 42.

As an aside, the variable N_n is simply used for notational simplicity. If you refer to it in conversation, people probably will not know what you are referring to, instead, you should call it “number of neutrons per decay”.

For anyone who would like to read further about making source terms, the Sources4c[14] and MISC[11] manuals has a complete mathematical description of (α, n) reactions, spontaneous fission, and delayed neutron sources. This reference has probably the most complete and understandable explanation of neutron sources.

4 Applications

Now that we have derived an equation to describe the evolution of a population of neutrons it is time to look at an application to familiarize ourselves with the properties of this equation. In particular, an important application in the context of nuclear reactors is neutron multiplication. In this section, we will use the transport equation to describe the criticality of a system.

The source-free ($q = 0$) neutron transport equation can be written in the form

$$\frac{1}{v} \frac{\partial \psi}{\partial t} = -\mathbf{\Omega} \cdot \nabla \psi - \sigma \psi + \int \int_{4\pi} \sigma' f' \psi' d\mathbf{\Omega}' dE' \quad (44)$$

Factoring out the v from each term, the right hand-side is a linear operation in N , hence we write

$$LN = -v\mathbf{\Omega} \cdot \nabla N - v\sigma N + \int \int_{4\pi} \sigma f' v' N' d\mathbf{\Omega}' dE'. \quad (45)$$

Next, we discuss how we can apply this representation of the neutron transport equation to a few application in the context of reactors.

4.1 α -eigenvalues

If we assume that there exists solutions of the form $N = \exp(\alpha t)N(\mathbf{x}, \mathbf{\Omega}, E)$, then Equation (44) becomes⁹

$$\alpha N(\mathbf{x}, \mathbf{\Omega}, E) = LN(\mathbf{x}, \mathbf{\Omega}, E). \quad (46)$$

As an aside, it is important to remember that the eigenvalue α is simply a mathematical construct, even though we are able to use the value of α to determine some physical properties of the system. In general, there exist many values of α 's satisfying Equation (46), so that we usually write

$$LN_j = \alpha_j N_j. \quad (47)$$

Equations of this form are called *eigenvalue* problems. For each j , Equation (47) determines an eigenvalue α_j of the linear (differential) operator L corresponding to an eigenfunction (solution) N_j .

We can use a neat trick with eigenvalues and eigenvectors. Namely, we can expand our solution to the original source-free equation (44) as an infinite series of the form

$$N = \sum_0^{\infty} \exp(\alpha_j t) N_j, \quad (48)$$

⁹For readers already familiar with the concept of eigenvalues, in general the eigenvalues of a linear operator may be complex. Hence, to be more thorough above, we need to replace α_0 above with $\text{Re}(\alpha_0)$, the real-part of the principal eigenvalue. Additionally, we have not addressed a few other related questions, e.g., convergence of the expression in (48). However, we will have to leave these important questions, which are outside the scope of this discussion, to more advanced texts.

using what is called the principle of superposition for linear operators. From Eqn. 48, we can draw a few important conclusions about the long time (or asymptotic) behavior of the neutron population in the system. Assuming that the eigenvalues are ordered so that $\alpha_0 > \alpha_1 > \alpha_2 > \dots$, then as $t \rightarrow \infty$, the behavior (growth versus decay) of the population is determined by the sign of the largest (principal) eigenvalue of the system. That is, as $t \rightarrow \infty$

$$N(\mathbf{x}, \mathbf{\Omega}, E, t) \approx C e^{\alpha_0 t} N_0(\mathbf{x}, \mathbf{\Omega}, E), \text{ as } t \rightarrow \infty, \quad (49)$$

where the value of C is determined from the initial conditions. Hence, there are three potential regimes we can say we are in:

1. If $\alpha_0 > 0$, the population is growing with time, and in the parlance of reactor theory we say that the system is *supercritical*.
2. If $\alpha_0 = 0$, then the population is steady in time, and we say that the system is *critical*.
3. If $\alpha_0 < 0$, the population is decreasing in time, and the system is called *sub-critical*.

Overall, the α -eigenvalue simply tells us how the neutron population is changing in time - does the population increase/stay the same/decrease in time?

4.2 The effective multiplication factor

The previous section taught us how to investigate the criticality of a time-dependent system. Here we consider the scenario when, for one reason or another, we have chosen not to solve the time-dependent problem, even through use of the α -eigenvalue. However, we still need to assess if our system is in a subcritical, critical, or supercritical state. We then choose to drop the time-dependent term in the neutron transport equation, Eqn. 44, which causes our balance equation to fall out of balance (since we are no longer accounting for how the neutron population changes in time). To re-balance the equation, we artificially rescale the fission term by $1/k$, and solve the resulting expression for the value of the k -eigenvalue. This provides a qualitative estimate of the system's critical state¹⁰¹¹. Starting from the steady-state transport equation in terms of N

$$\frac{1}{v} \frac{\partial \psi}{\partial t} + \mathbf{\Omega} \cdot \nabla \psi + \sigma(\mathbf{x}, E) \psi = \int \int_{4\pi} \sigma_s f'_s \psi' d\mathbf{\Omega}' dE' + \chi(E) \int \frac{\nu'}{k} \sigma'_f \int_{4\pi} \psi' d\mathbf{\Omega}' dE' + q(\mathbf{x}, \mathbf{\Omega}, E, t), \quad (50)$$

where the factor k is called an effective multiplication factor or k -effective eigenvalue. The assumption behind including the multiplication factor k is that, any fissile material can be made critical by adjusting the number of neutrons emitted per fission. There are three conditions that can occur:

1. $k > 1$ in a supercritical system in order to reduce the number of neutrons emitted per fission so that the solution appears to be steady.
2. $0 < k < 1$ in a sub-critical system in order to increase the number of neutrons emitted per fission to maintain a stationary population.

¹⁰We consider the k -eigenvalue to be a qualitative judgement, because the value of k only leads to high level qualitative statements. Take two systems, the first with a k value of 0.8 and the second with a k value of 0.4. You know that both systems are subcritical and the second system is more subcritical than the first. However, the k -eigenvalue is insufficient to make any quantitative conclusions about the neutron population between the two systems (i.e., the neutron population in the second system is half as much as in the first system.)

¹¹The benefit of the k -eigenvalue problem is that it is sometimes easier to solve than the alpha-eigenvalue one, even if most such solutions feature less physical fidelity.

3. $k = 1$ is the steady-state case, or the critical system.

Again, the k eigenvalue term is a mathematical construct used to force the system into a critical state. One way to find the value of k relies on turning Eqn. 50 into an eigenvalue problem.

To express Equation (50) in terms of a linear operator that defines the eigenvalue spectrum for k requires a some additional work. First, we express the *multiplication* term using

$$MN = v \int \int_{4\pi} \sigma f' N' d\Omega' dE', \quad (51)$$

and the *transport* terms using

$$TN = v\mathbf{\Omega} \cdot \nabla N + v\sigma N, \quad (52)$$

Then we can write Equation (50) in terms of linear transformations as

$$TN = \frac{1}{k}MN. \quad (53)$$

Rearranging, we can have

$$T^{-1}MN_j = k_j N_j. \quad (54)$$

As before, there exist many values of k satisfying Equation (53), and in general these values are called the spectrum of eigenvalues defined by the eigenvalue problem in Equation (54).

So far we have just covered a couple applications of the neutron transport equation which can be used to determine if a system is critical or not. However, we still have not attempted to solve the neutron transport equation. That is because solving this equation is actually impossible in all but the most simple of systems¹². The next section will cover some approximation methods for solving the neutron transport equation, Eqn. 40.

5 Approximations

The integral term on the right hand side of Equation (37) combining the contributions to the neutron population through scattering and possibly fission mathematically categorizes it as a non-local, integro-differential equation. This is in contrast to other familiar conservation laws as local or pointwise in the form of standard partial differential equations. The difference here is a consequence of the fact that, for example in the case of scattering, incident neutrons from any angle $\mathbf{\Omega}'$ may produce a neutron traveling in any given direction $\mathbf{\Omega}$. Hence, as we saw in our derivation, we must integrate over all possible incoming angles for each possible outgoing angle. This is non-local in the sense that the outgoing angle is not assumed to be a continuous function of the incoming angle.

All of the forthcoming approximation methods to the neutron transport equation that we will discuss are developed to achieve essentially the same goal. Namely, to approximate the integral terms as finite sums across discrete partitions of the integrand. In particular, this reduces the neutron transport equation mathematically from an integro-differential equation to a more tractable coupled system of partial differential equations. Although both simplifications we discuss below are helpful in the analysis of the transport equation, they are also usually the first step to building a numerical method to solve the transport equation in more specialized applications. Although we will not discuss the topic of numerical methods for the transport equation here the interested reader can find a comprehensive treatment of several widely-used numerical methods in [9].

¹²The transport equation is integro-differential equation, easily one of the hardest types of equations in mathematics to solve. To complicate the matter further, the neutron transport equation depends on seven variables (3 spatial, 2 directional, energy, and time), but at least the equation is linear! However, the transport equation can be solved in a pure absorbing material - a material where the only possible interaction is neutron absorption. Duderstadt and Hamilton provide an example of solving the transport equation in a pure absorber [4]. In any other system, the only way to solve the neutron transport equation exactly is to perfectly guess the solution to the flux. Good luck!



Figure 6: We discretize the energy range into groups where group 1 is the highest energy and group G is the lowest energy.

5.1 The multigroup equations

Starting from the steady-state (time-independent) form of the neutron transport equation for simplicity¹³, similar to Equation (40):

$$(\mathbf{\Omega} \cdot \nabla + \sigma)\psi = q + \int_0^\infty \int_{4\pi} \sigma'_s f'_s \psi' d\mathbf{\Omega}' dE' + \chi(E) \int_0^\infty \nu' \sigma'_f \int_{4\pi} \psi' d\mathbf{\Omega}' dE', \quad (55)$$

the neutron energy spectrum is discretized into G subintervals called energy groups, Fig. 6. By convention, the lowest energy group corresponds to index G and is defined by the interval $0 \leq E < E_{G-1}$. The highest energy group then defined by $E_2 \leq E < E_1$, where E_1 is chosen sufficiently high so that the number of neutrons with energy higher than E_1 is negligible.

Next, for each group g , we introduce a new quantity called the *group angular flux*, defined by

$$\psi_g(x, \mathbf{\Omega}) = \int_g \psi dE, \quad (56)$$

where the integral over each group is defined by

$$\int_g dE = \int_{E_g}^{E_{g-1}} dE. \quad (57)$$

The energy integrals in Equation (55) can then be approximated by the contributions from each energy group by the sum¹⁴

$$\int_0^\infty dE \approx \sum_{g=1}^G \int_g dE. \quad (58)$$

Next, Equation (55) integrated over an energy group E_g becomes

$$\begin{aligned} \mathbf{\Omega} \cdot \nabla \int_g \psi dE + \int_g \sigma \psi dE &= \int_g q dE + \int_g \sum_{g'=1}^G \int_{g'} \int_{4\pi} \sigma'_s f'_s \psi' d\mathbf{\Omega}' dE' dE \\ &+ \int_g \chi(E) \sum_{g'=1}^G \int_{g'} \nu' \sigma'_f \int_{4\pi} \psi' d\mathbf{\Omega}' dE' dE \end{aligned} \quad (59)$$

after applying the approximation in (58).

Energy separability

In order to obtain the multigroup equations, we make the assumption that within each group E_g , the angular flux can be expressed as a product of the form

$$\psi(x, \mathbf{\Omega}, E) = h(E) \psi_g(\mathbf{x}, \mathbf{\Omega}), \quad E_g < E < E_{g-1}, \quad (60)$$

¹³The same concepts applied here can be used to develop a time-dependent multigroup formulation of the transport equation as well.

¹⁴This is simply the rectangle rule that you learned to approximate integrals in your calculus I class.

where the known function h is called the *energy-dependent spectral weighting function*. In most cases the spectral weighting function h is assumed to be normalized over each group g so that

$$\int_g h(E) dE = 1. \quad (61)$$

Substituting (60) with (61) into (59) yields

$$\begin{aligned} \mathbf{\Omega} \cdot \nabla \int_g h(E) \psi_g dE + \int_g \sigma h(E) \psi_g dE &= q_g + \int_g dE \sum_{g'=1}^G \int_{4\pi} d\mathbf{\Omega}' \int_{g'} dE' \sigma'_s f'_s h(E) \psi_{g'} \\ &+ \int_g dE \chi(E) \sum_{g'=1}^G \int_{g'} dE' \nu' \sigma'_f \int_{4\pi} d\mathbf{\Omega}' h(E) \psi_{g'}. \end{aligned} \quad (62)$$

The ultimate and penultimate terms on the right hand side of Equation (62) motivate the definition of the *multigroup cross section* given by

$$\sigma_g = \int_g h(E) \sigma dE. \quad (63)$$

Expressing Equation (62) in terms of the multigroup cross-section, we obtain

$$\begin{aligned} \mathbf{\Omega} \cdot \nabla \psi_g + \sigma_g \psi_g &= q_g + \sum_{g'=1}^G \int_{4\pi} (\sigma'_s f'_s)_{g'} \psi_{g'} d\mathbf{\Omega}' \\ &+ \int_g \chi(E) \sum_{g'=1}^G (\nu \sigma'_f)_{g'} \int_{4\pi} \psi_{g'} d\mathbf{\Omega}' dE. \end{aligned} \quad (64)$$

From which we then obtain the conventional multi-group form of the steady-state transport equation:

$$\begin{aligned} (\mathbf{\Omega} \cdot \nabla + \sigma_g) \psi_g &= \sum_{g'=1}^G \int_{4\pi} (\sigma'_s f'_s)_{g'} \psi'_{g'} d\mathbf{\Omega}' \\ &+ \int_g \chi(E) \sum_{g'=1}^G (\nu \sigma'_f)_{g'} \int_{4\pi} \psi_{g'} d\mathbf{\Omega}' dE + q_g. \end{aligned} \quad (65)$$

This process has removed the integral over E , but it came at a cost. We now have a set of G coupled integro-differential equations to solve. It may not be obvious to see what we have gained by creating the multigroup equations but hopefully it becomes more obvious once we handle the integral over $\mathbf{\Omega}$ in Sec. 5.4.

5.2 One-group transport equation

The multi-group equations in (65) can be thought of individually as an equation describing the evolution of the packet of neutrons with energy E_g . The simplest case would be the reduction to one energy group; this is usually called the *one-speed transport equation*. In many cases, this assumption may over simplify systems, however, it's important to discuss from a mathematical point of view since solving a system of multi-group equations requires solving G coupled, one-speed equations.

If we assume one energy group to describe the entire population, returning to the steady state version of the neutron transport equation in (55), the cross sections and angular flux no longer depend on energy, and we can start our derivation from the form:

$$(\mathbf{\Omega} \cdot \nabla + \sigma) \psi(\mathbf{x}, \mathbf{\Omega}) = \int \int_{4\pi} \sigma' f' \psi' d\mathbf{\Omega}' dE'. \quad (66)$$

The right hand side can then be expanded as

$$\begin{aligned}\int \int_{4\pi} \sigma' f' \psi' d\Omega' dE' &= \int \int_{4\pi} \sum_x \sigma'_x f'_x \psi' d\Omega' dE' \\ &= \sum_x \int \int_{4\pi} \sigma'_x f'_x \psi' d\Omega' dE'\end{aligned}\quad (67)$$

Using the fact that the angular flux and cross sections are independent of energy E , that is, $\sigma_x(\mathbf{x})$ and $\psi(\mathbf{x}, \Omega)$, respectively, we have

$$(\Omega \cdot \nabla + \sigma)\psi(\mathbf{x}, \Omega) = \sum_x \sigma'_x \int_{4\pi} \psi' \int f'_x dE' d\Omega'. \quad (68)$$

Since the angular distribution of neutrons emitted in any collision must also be independent of energy $\int f'_x(\Omega' \rightarrow \Omega, E' \rightarrow E) dE' = c_x f'_x(\Omega' \rightarrow \Omega)$, we can further condense the right hand side to

$$\begin{aligned}\sum_x \sigma'_x \int_{4\pi} \psi' \int f'_x dE' d\Omega' &= \sum_x \sigma'_x \int_{4\pi} \psi' c_x f'_x(\Omega' \rightarrow \Omega) d\Omega' \\ &= \sum_x c_x \sigma'_x \int_{4\pi} f'_x(\Omega' \rightarrow \Omega) \psi' d\Omega',\end{aligned}\quad (69)$$

where c_x denotes the mean number of neutrons emitted by reaction type x . For example, for scattering and fission reactions $c_s = 1$ and $c_f = \bar{\nu}$ neutrons, respectively, and $c\sigma = (\sigma_s + \bar{\nu}\sigma_f)$. We can write the previous more compactly by denoting

$$c\sigma \int_{4\pi} f'(\Omega' \rightarrow \Omega) \psi' d\Omega' = \sum_x c_x \sigma'_x \int_{4\pi} f'_x(\Omega' \rightarrow \Omega) \psi' d\Omega'. \quad (70)$$

Finally, we can write the one-speed transport equation in the form

$$(\Omega \cdot \nabla + \sigma)\psi(\mathbf{x}, \Omega) = c\sigma \int_{4\pi} f'(\Omega' \rightarrow \Omega) \psi(\mathbf{x}, \Omega' \rightarrow \Omega) d\Omega'. \quad (71)$$

In the next section, we will digress into geometric reductions before we approximate the remaining integral (with respect to angle) in Equation (71) over a discrete (finite) set of angles. In the case of the latter, the neutron transport equation will be reduced to a linear system of PDEs, which is much more tractable relatively speaking.

5.3 Geometric Approximations

Solving the 3D form of the neutron transport equation, even the monoenergetic form in Eqn. 71, is very challenging. However, a common approach is to consider the geometry of one's problem and make appropriate approximations to the problem geometry in turn. These are our geometric approximations. Namely, we will show how to make the 1D planar form of Eqn. 71. Before applying these assumption, we will describe approaches for determining when we can use them¹⁵.

In general, we would like to solve 1D equations if we can justify this decision. There is no one size fits all approach for determining when a problem can be reduced from 3D to 1D, however, we often make consolations in order to arrive at tractable equations. Some indicators to look for when reducing the complexity of the problem are:

¹⁵Reducing the complexity of the geometry is a helpful method for solving difficult problems. When appropriately applied these approximations can yield an accurate result while simultaneously reducing the time it takes to solve a problem. However, if inappropriately applied, these methods will give drastically incorrect answers.

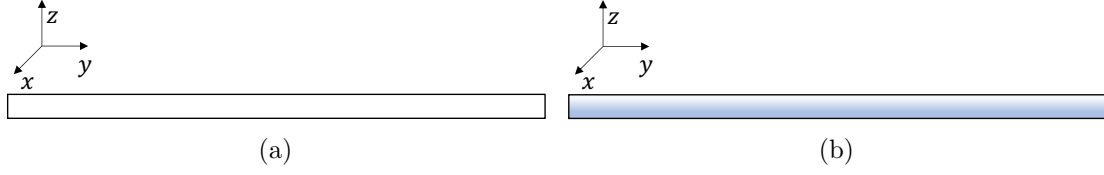


Figure 7: (a) shows a slab that is taken to be much longer in the x- and y- directions than in the z-direction. Therefore, we can reduce the geometry of the problem and account only for the z-direction. (b) the slab in this image has a constant varying density along the z-direction, but constant density in the x- and y- directions. Therefore, we can reduce the problem keeping only the z-dependence.

1. one or more dimensions of an object are much greater than the remaining dimension(s)
2. some property of an object varies much more slowly along one or more dimensions as compared to how the same quantity varies in the remaining dimension(s)
3. the geometry of a problem is well suited for a curvilinear treatment over a Cartesian treatment

The first item in the list refers to objects that are longer in one or two dimensions but thin in the remaining dimension(s), shown in Fig. 7a. This slab is much long in the x- and y-directions than in the z-direction. Hence, we can neglect the x- and y- directions and solve the problem in 1D, along the z-direction. The second item refers to Fig. 7b, where the density of slab is changing along the z-direction but remains constant along the x- and y-directions. Here we can neglect the x- and y-directions again since there is little variation in the density along the x- and y-directions as compared to the density variation along the z-direction. The final item refers to the geometry shape of an object. If an object resembles a cylinder or sphere, it is conducive to use cylindrical or spherical coordinates to express our equations¹⁶.

1D Planar

Now that we have determined when it is appropriate to apply a geometric approximation, we need to reduce our equations. Reducing the problem from three spatial dimensions to one spatial dimension eliminates two of the three spatial derivatives in Eqn. 71 and one of the two direction derivatives. As an aside, the components of the direction vector $\hat{\Omega}$ are ϕ ¹⁷ and θ components, shown in Fig. 8. ϕ is the azimuthal angle and θ is the polar angle. It is common to define the variable μ in terms of θ as

$$\mu \equiv \cos \theta, \quad (72)$$

where μ is defined over the range $[-1, 1]$ and ϕ is defined over the range $[0, 2\pi]$.

Integrating Eqn. 71 over y, z, and ϕ reduces the dimensionality of the problem as

$$\int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \left[(\Omega \cdot \nabla + \sigma) \psi(\mathbf{x}, \Omega) = c \sigma \int_{4\pi} f'(\Omega' \rightarrow \Omega) \psi(\mathbf{x}, \Omega' \rightarrow \Omega) d\Omega' \right]. \quad (73)$$

¹⁶This should remind you of your calculus class. If you need a refresher on these coordinate systems grab your favorite calculus text book or you can look at [6]

¹⁷It may seem confusing to have another ϕ show up. However, we usually consider the flux to be symmetric about the azimuthal angle, and therefore, neglect the azimuthal angle quite frequently. We can make this assumption because nuclear interactions tend to be invariant about the azimuthal angle.

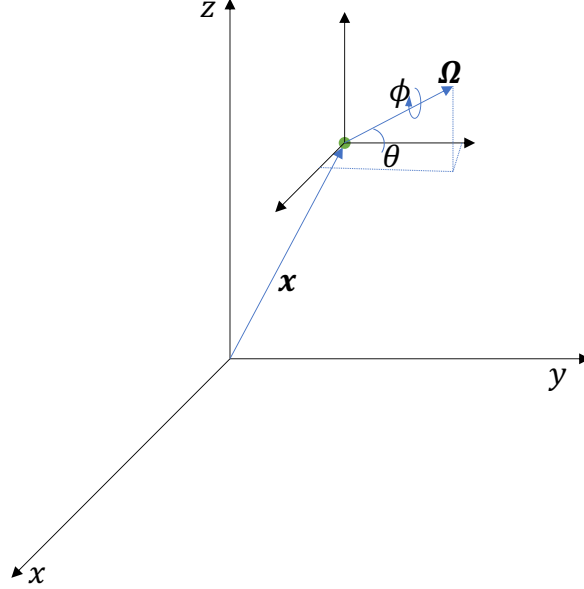


Figure 8: The components of Ω , where ϕ is the azimuthal angle and θ is the polar angle.

Then, evaluating the integrals over dy and dz yields:

$$\left(\mu \frac{d}{dx} + \sigma\right) \psi(x, \mu) = \frac{c\sigma}{2} \int_{-1}^1 f'(\mu' \rightarrow \mu) \psi(x, \mu' \rightarrow \mu) d\mu', \quad (74)$$

where the factor 2π is a consequence of changing the bounds of integration from $d\Omega'$ to $d\mu'$ and x represents our one remaining spatial variable.

Eqn. 74 is the steady-state 1D planar form of the neutron transport equation. While this equation appears much simpler to solve, the derivative on the left-hand side and remaining integral on the right-hand side indicate the equation is still an integro-differential equation and further simplification is required to arrive at a tractable form. Now that we have shown how to derive the 1D form of the neutron transport equation, it is important to identify a method for choosing when this form can be used.

Deciding when to apply geometric reductions is a useful skill. One way to determine if a problem can be reduced from one coordinate system to a less complex coordinate system is to compare non-dimensionalized forms of an equation in both coordinate systems. Here we will provide an example of this process using the diffusion equation, which will be derived in Sec. 5.5. While we have not yet introduced the diffusion equation, it acts as a simple and clear example problem for this process. We will use the diffusion equation to see at what radius value we can switch from using a 1D cylindrical equation to a 1D planar equation.

Non-dimensional analysis is a process where an equation is rewritten in a manner such that there are no units in the problem (i.e., all parameters and variables in an expression are redefined using ratios rather than dimensional quantities). Starting with the geometry-independent diffusion equation,

$$-D\nabla^2 \phi + \Sigma_a \phi = q. \quad (75)$$

where the second derivative has been written using the gradient, D is the diffusion coefficient, ϕ is the scalar flux, Σ_a is macroscopic absorption cross section, and q is the source term. The monoenergetic, steady-state, 1D planar diffusion approximation:

$$-D \frac{d^2 \phi}{dx^2} + \Sigma_a \phi = q. \quad (76)$$

Dividing the equation by $-D$ and defining $L^{-2} \equiv \frac{\Sigma_a}{D}$,

$$\frac{d^2\phi}{dx^2} - \frac{1}{L^2}\phi + \frac{q}{D} = 0. \quad (77)$$

Non-dimensionalizing x ,

$$\tilde{x} = \frac{x}{L}, \quad (78)$$

where \tilde{x} is the non-dimensionalized form of x . The first derivative becomes

$$dx = L d\tilde{x} \quad (79)$$

in non-dimensional form.

The second order differential of x , dx^2 , becomes

$$dx^2 = L^2 d\tilde{x}^2. \quad (80)$$

Eqn. 76 then becomes

$$\frac{1}{L^2} \frac{d^2\phi}{d\tilde{x}^2} - \frac{1}{L^2}\phi + \frac{q}{D} = 0, \quad (81)$$

or,

$$\frac{d^2\phi}{d\tilde{x}^2} - \phi + \frac{L^2 q}{D} = 0. \quad (82)$$

Note: $\frac{L^2 q}{D}$ has units of $Length^{-2}Time^{-1}$, which are the same units as ϕ . So,

$$\tilde{\phi} = \frac{\phi}{L^2 q / D}, \quad (83)$$

or,

$$\phi = \tilde{\phi} \frac{L^2 q}{D}, \quad (84)$$

where $\tilde{\phi}$ is the non-dimensionalized form of ϕ . The second differential of ϕ becomes

$$d^2\phi = \frac{L^2 q}{D} d^2\tilde{\phi}. \quad (85)$$

Using $\tilde{\phi}$, Eqn. 82 is written as

$$\frac{L^2 q}{D} \frac{d^2\tilde{\phi}}{d\tilde{x}^2} - \frac{L^2 q}{D} \tilde{\phi} + \frac{L^2 q}{D} = 0, \quad (86)$$

or,

$$\frac{d^2\tilde{\phi}}{d\tilde{x}^2} - \tilde{\phi} + 1 = 0. \quad (87)$$

The 1D planar diffusion approximation is now expressed in a non-dimensional form.

Expressing the gradient in Eqn. 76 in 1D cylindrical coordinates yields

$$\frac{1}{r} \frac{d}{dr} \left(r \frac{d\phi}{dr} \right) - \frac{1}{L^2}\phi + \frac{q}{D} = 0, \quad (88)$$

or,

$$\frac{d^2\phi}{dr^2} + \frac{1}{r} \frac{d\phi}{dr} - \frac{1}{L^2}\phi + \frac{q}{D} = 0. \quad (89)$$

Let

$$\tilde{r} = \frac{r}{L}, \quad (90)$$

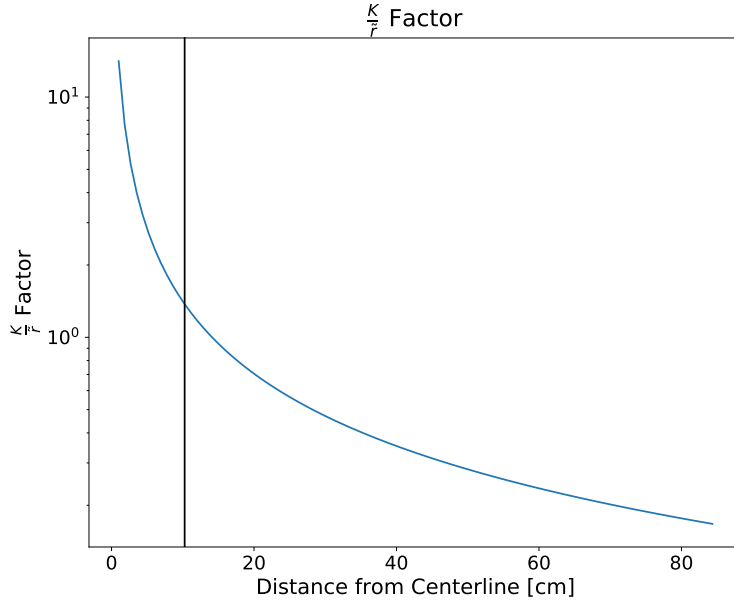


Figure 9: As the factor $\frac{k}{\tilde{r}}$ decreases, the planar solutions better approximate cylindrical solutions. The location of the black vertical line shows the point where the factor $\frac{k}{\tilde{r}}$ is 10% of its initial value at $r = 10.26$ cm.

and,

$$\tilde{\phi} = \frac{\phi D}{L^2 q} \quad (91)$$

Using the non-dimensionalized variables defined in Eqns. 90 and 91, Eqn. 89 can be rewritten as

$$\frac{d^2 \tilde{\phi}}{d\tilde{r}^2} + \frac{1}{\tilde{r}} \frac{d\tilde{\phi}}{d\tilde{r}} - \tilde{\phi} + 1 = 0. \quad (92)$$

Then, the curvilinear form of the diffusion equation is

$$\frac{d^2 \tilde{\phi}}{d\tilde{r}^2} + \frac{k}{\tilde{r}} \frac{d\tilde{\phi}}{d\tilde{r}} - \tilde{\phi} + 1 = 0, \quad (93)$$

where $k = 0$ for planar geometries and $k = 1$ for cylindrical geometries. Further, plotting the variable $\frac{k}{\tilde{r}}$ for $k = 1$ will show the location where accounting for cylindrical geometries becomes negligible. Figure 9 shows the result from the previous dimensional analysis using material properties of the fuel materials. The black vertical line in Fig. 9 shows the location where the value of $1/\tilde{r}$ (since $k = 1$ in cylindrical) is 1.41, or 10% of its initial value (14.11). The location of the vertical black line shows where the cylindrical and planar models agree within 90%, and is located at 10.26 cm. After 10.26 cm materials can be approximated using planar equations. The value of 10% is somewhat arbitrary in this example, and you may find that you need to increase or decrease this cutoff value depending on how accurate your results need to be for a given application.

By no means is the previous methodology your only approach to determining the feasibility of using a geometric approximation. Rather, it demonstrates one good trick to have when someone asks you to defend your reasoning for reducing the geometric complexities of your problem. From here, we will discuss how to handle the remaining integral term, the integral over μ , in Eqn. 74.

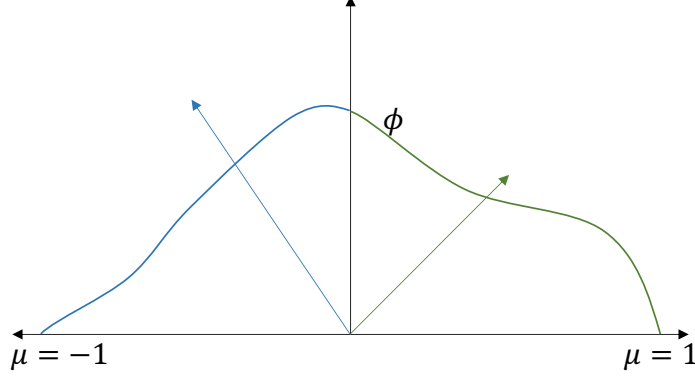


Figure 10: The green and blue curvy lines represent some neutron flux angular distribution over a continuum of directions. The discrete ordinates method instead treats the neutron flux at a set of discrete angles given by the arrows, where the discrete flux corresponds to a continuous flux based on the color.

5.4 Angular discretization

In the previous sections, we introduced the multi-group approximation to approximate the energy integrals as well as how to reduce the number of spatial derivatives present in the neutron transport equation. In this section, our goal is to approximate the remaining integral on the right hand side by discretizing the variable specifying the direction variable into *angular packets*. Our starting point will be the one-speed planar approximation in Equation (74). Recall that the system of multi-group equations is simply a coupled version of the one-speed equation. Hence, if we can successfully achieve our goal for the one-speed equation, –presto, we can solve G equations by applying the same technique repeatedly.

So far we have been trying to reduce the integrals present in the neutron transport equation into something that we can handle. For all of our hard work and assumptions, we still have one more integral term left to handle, namely the integral over direction. We could handle this by assuming the neutron flux is isotropically distributed, but that would be a stretch to consider. Instead, we choose a more robust assumption, we assume that the continuous directional dependence can be approximated using a finite sum over a discrete set of directions. This is called the discrete ordinate (or discrete direction) approximation. We begin by taking the steady-state, one-speed, 1D planar transport equation. In planar coordinates, the neutron transport equation (Eqn. 74) with an external source term written in terms of the angular flux is given by

$$\mu \frac{\partial \psi}{\partial x} + \sigma \psi = \frac{\sigma(x)c(x)}{2} \int_{-1}^1 \psi' d\mu' + q. \quad (94)$$

Discrete ordinates treats directional dependence by evaluating the integral over μ at a unique set of directions, $\{\mu_i\}$. Evaluating the integral in Eqn. 94 at each value of μ_i leads to a weighted sum of neutron fluxes, Eqn.

$$\int_{-1}^1 \psi' d\mu' = \sum_{i=1}^M w_i \psi(x, \mu_i), \quad (95)$$

where w_i are the weights corresponding to the directions μ_i , then (94) becomes

$$\mu_i \frac{\partial \psi_i}{\partial x} + \sigma \psi_i = \sigma(x) \frac{c(x)}{2} \sum_{i=1}^M w_i \psi_i + q. \quad (96)$$

for $i = 1, 2, \dots, M$. This system of M equations can then be solved for the evolution of each direction-packet corresponding to $\psi_i(x) = \psi(x, \mu_i)$. While nothing has been said about requirements for selecting the directions $\mu_{ii} = 0^M$ and weights $w_{ii} = 0^M$, two general requirements are

1. Since the angular flux is always positive, $w_i > 0$.
2. The choice of directions and weights should be symmetric, $\mu_i = -\mu_{M-i+1}$ and $w_i = w_{M-i+1}$.

The second rule requires an even choice of M . If M were taken to be odd, one value of μ would fall on 0. This creates a problem since the direction cosine at $\mu = 0$ is perpendicular to the x-axis and the derivative term in Equation 96 would vanish. Another problem occurs when finding the flux at a vacuum boundary using $\mu = 0$. One would expect a non-zero flux leaving the material and a zero flux entering the material from the vacuum. The discrepancy in the flux at the material-vacuum interface leads to a discontinuity if μ is evaluated at 0.

A third property that to be considered is that if ψ is approximated well by a low-order polynomial, then our quadrature rule, Equation (95), should be exact. For example, using weights and nodes defined which yield a Gaussian-Legendre quadrature rule¹⁸.

5.5 The diffusion equation

Here we develop a common approximation to the transport equation called the diffusion equation. The diffusion equation is considered a foundational equation in nuclear engineering and it tends to be the first approximation to the transport equation that students are taught in universities. The diffusion equation assumes the neutron flux as at most linearly anisotropic and slowly varying in time (slowly varying in comparison to the time between neutron interactions). While the diffusion equation may seem limited in complexity, this equation is actually commonly used in reactor theory. We begin our derivation with Eqn. 96 where we take two directions, or $i = 2$. Together, these two equations are called the monoenergetic S_2 equations without an external source,

$$\mu_1 \frac{\partial \psi_1}{\partial x} + \sigma \psi_1 = \frac{c(x)\sigma(x)}{2}(\psi_1 + \psi_2) \quad (97)$$

$$-\mu_1 \frac{\partial \psi_2}{\partial x} + \sigma \psi_2 = \frac{c(x)\sigma(x)}{2}(\psi_1 + \psi_2). \quad (98)$$

We have assumed a monoenergetic formulation of the Eqn. 96, however that is not a necessity, and these equations could easily be extended to include a multigroup energy-dependence. Further, μ_2 has been substituted for $-\mu_1$. In fact, μ_1 has to be equal in value and opposite in sign from μ_2 in order for the S_2 equations to be equivalent to the diffusion approximation¹⁹. In the S_2 approximation the scalar flux, ϕ and the current, J , are defined as

$$\phi \equiv \frac{1}{2}(\psi_1 + \psi_2) \quad (99)$$

$$J \equiv \frac{1}{2}\mu_1(\psi_1 - \psi_2). \quad (100)$$

¹⁸Gaussian-Legendre quadrature is just a fancy (and common) way of choosing the angles of your direction vectors. You don't have to use a Gaussian-Legendre quadrature if there is something about your problem that would indicate choosing a different set of direction vectors. More is said about Gaussian-Legendre quadrature in [9].

¹⁹In the case where μ_1 and μ_2 are equal and opposite in value, the two directions are spread evenly across the direction space. Put another way, the two direction vectors are as far apart as possible. Doing so, evenly samples the direction space, which is a good first guess when you have no indicators of how the flux looks.

In general, many systems of two first-order ordinary differential equations can be written as a single second-order differential equation. In fact, that is what we want to do here in order to develop the diffusion approximation. First, by adding Eqns. 97 and 98 and using definitions 99 and 100 yields

$$\mu_1 \frac{\partial \psi_1}{\partial x} - \mu_1 \frac{\partial \psi_2}{\partial x} + \sigma(\psi_1 + \psi_2) = c(x)\sigma(\psi_1 + \psi_2), \quad (101)$$

or,

$$\mu_1 \left(\frac{\partial(\psi_1 - \psi_2)}{\partial x} \right) + \sigma(\psi_1 + \psi_2) - c(x)\sigma(\psi_1 + \psi_2), \quad (102)$$

such that,

$$2 \frac{\partial J}{\partial x} + 2\sigma\phi - 2c(x)\sigma\phi = 0 \quad (103)$$

or,

$$\frac{\partial J}{\partial x} + (\sigma - c(x)\sigma)\phi = 0, \quad (104)$$

and defining $\sigma - c(x)\sigma = \sigma_a$ yields,

$$\frac{\partial J}{\partial x} + \sigma_a\phi = 0. \quad (105)$$

By subtracting Eqns. 97 and 98 and using definitions 99 and 100,

$$\mu_1 \frac{\partial \psi_1}{\partial x} + \mu_1 \frac{\partial \psi_2}{\partial x} + \sigma(\psi_1 - \psi_2) = 0, \quad (106)$$

such that,

$$\mu_1 \frac{\partial}{\partial x}(\psi_1 + \psi_2) + \sigma(\psi_1 - \psi_2) = 0, \quad (107)$$

multiplying by μ_1 ,

$$\mu_1 \sigma(\psi_1 - \psi_2) = -\mu_1^2 \frac{\partial \phi}{\partial x}, \quad (108)$$

which simplifies to,

$$J\sigma = -\mu_1^2 \frac{\partial \phi}{\partial x}. \quad (109)$$

Eqn. 109 is equivalent to Fick's Law²⁰ when $\mu_1 = \frac{1}{\sqrt{3}}$, which is true when using Gaussian-Legendre quadrature. Upon substituting Eqn. 109 into Eqn. 105 results in the diffusion equation,

$$\frac{\partial}{\partial x} \left(\frac{-\mu_1^2}{\sigma} \frac{\partial \phi}{\partial x} \right) + \sigma_a\phi = 0. \quad (110)$$

Commonly, we set D , or the diffusion coefficient, equal to $-\mu_1^2/\sigma$ such that Eqn. 110 can be rewritten as

$$-D \frac{\partial}{\partial x} \left(\frac{\partial \phi}{\partial x} \right) + \sigma_a\phi = 0. \quad (111)$$

As a reference, if we are to extend Eqn. 111 into three dimensions, we need to invoke the use of the Laplacian operator. Doing so lets us arrive at the more general 3D diffusion approximation,

$$-D (\nabla^2 \phi) + \sigma_a\phi = 0. \quad (112)$$

This form of the diffusion equation is helpful when a problem requires the use of a curved geometry since the Laplacian operator can be expressed in Cartesian, cylindrical, or spherical forms. In the previous derivation, four assumptions are made which must be adhered to in order for the S_2 equations and diffusion approximation to be equivalent:

²⁰Fick's Law commonly shows up when solving any type of diffusion equation. In fact, the neutron diffusion equation gains its name from treating the neutrons like a specimen diffusion through a medium just like in heat transfer, chemistry, and other areas of science and engineering.

1. μ_1 and μ_2 must be chosen symmetrically, i.e. have the same value but opposite signs;
2. $\mu_1 = -\mu_2 = \frac{1}{\sqrt{3}}$ if the S_2 equations are to have the traditional definition for the diffusion coefficient;
3. $\sigma \neq 0$, i.e. this derivation will not hold in void;
4. The material must be homogenous.

The first three assumptions must be satisfied in order for these equations to be equivalent, however, the fourth condition can be relaxed by treating both the diffusion coefficient and the cross sections as functions of position during their respective derivations.

The diffusion equation is known to suffer inaccuracies when

1. The neutron flux is not isotropic which violates assumption 1 in the previous list,
2. When the material is highly absorbing which violates assumption 2 in the previous list
3. Near material boundaries which violates assumption 4 in the previous list.

While these criteria may seem constrictive, the diffusion equation is often used to approximate the neutron flux even when one, or all three, of these assumptions are broken!

Further reading

Lamarsh and Baratta [7] is considered a great resource for matters which use the diffusion equation. In this authors' opinion, Lewis [8] provides the most basic description of some of the concepts we have described in this section. For multigroup and discrete ordinates discussion, the author believes that Duderstadt and Hamilton [4] and Bell and Glasstone [1] have the best descriptions of the multigroup discrete ordinates approximations, the techniques used for angular and energy discretization.

6 Example problems

In this section, we will show two example problems to help the reader practice the theories we have introduced.

1D polar diffusion problem

The first example uses the diffusion equation in a cylindrical neutron source material (i.e.; non-zero fission cross section) surrounded by a vacuum, Fig. 11. We will also assume there is some initial source, q , of neutrons in the material. We will tackle this problem in 1D. The 1D radial²¹ form of Eqn. 112 arrives from using the 1D radial definition of the Laplacian operator as

$$\frac{-D}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \phi}{\partial r} \right) + \sigma_a \phi = \bar{\nu} \sigma_f \phi + q, \quad (113)$$

where $\bar{\nu}$ is the average number of neutrons emitted per fission, σ_f is the fission cross section, σ_a is the absorption cross section, and q is our neutron source term. Here, we need to use the polar form of the diffusion equation given the curvilinear geometry of the problem.

²¹You may be wondering what a 1D radial system would like. Think about an infinitely long cylinder. You would expect to see some variation in the neutron flux as you moved from the center of the cylinder radially outward to the edge. Alternatively, there would be little change in the neutron flux if you moved up and down the length of the cylinder. This is what is meant by 1D radial. In reality, a 1D radial system would look like a thin but long cylinder, something like a fuel rod used in a nuclear reactor. As long as you stay away from the edges of the rod, the neutron flux only has small variations as a function of length.

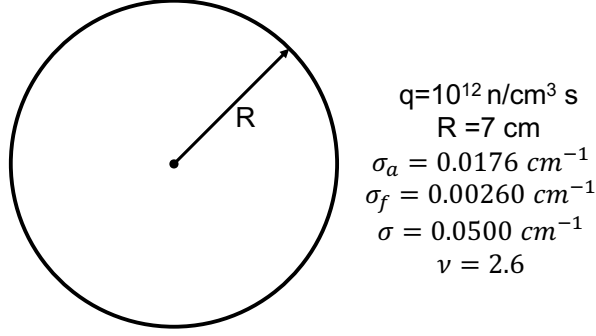


Figure 11: This example looks at a multiplying material which contains a neutron source in radial geometry. We want to find the neutron flux as a function of radius in the material.

If we divide Eqn. 113 by $-D$ and combine like terms,

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \phi}{\partial r} \right) - \phi \left(\frac{\sigma_a - \bar{\nu} \sigma_f}{D} \right) + \frac{q}{D} = 0. \quad (114)$$

To solve equation 114, we define the variable B as:

$$B^2 \equiv \frac{\sigma_a - \bar{\nu} \sigma_f}{D}. \quad (115)$$

The term B is called the material buckling²² term since it depends on material properties only. Various authors write about the material buckling for the interested reader [4, 7, 8]. We know the general solution to a problem of the form in Eqn. 114 with the definition of the material buckling provided in Eqn. 115 to be [6]

$$\phi = AI_0(Br) + CK_0(Br) \text{ with } A \text{ and } C = \text{constants}, \quad (116)$$

where I_0 and K_0 are modified Bessel functions²³ of the first and second kind respectively. To solve for the constants, A and C , we set the boundary conditions from the definition of our problem to be:

1. Flux at $r = 0$ is finite, $\phi(r = 0) < \infty$,
2. Flux is zero at an extrapolated radius, $\phi(r = \tilde{R}) = 0$, since the system is in a vacuum.

Here we have chosen the flux to go to 0 at the extrapolated radius. The extrapolated radius is a mathematical construct that “adjusts” the value of the neutron flux near the boundary of a material. If you recall, the diffusion equation fails near material boundaries. The extrapolated radius adjusts the flux at the boundary to account for deficiencies in using the diffusion equation. Lamarsh and Baratta provide an excellent description of the extrapolated boundary condition [7]. It will suffice us for now to say that the extrapolated radius is defined as

$$\tilde{R} = R + 2.13D. \quad (117)$$

Applying the first boundary condition sets $C = 0$, since K_0 goes to infinity as r goes to zero. The second constant, A , is found by solving the homogenous and inhomogeneous equations for

²²Way back when someone thought this term resembled a beam buckling equation encountered in structural mechanics, hence the name “buckling”... or so the rumor goes.

²³Bessel functions are an example of a special function. These functions are a solution to Bessel’s differential equations. They are related to cylindrical and spherical harmonics. If you are interested in Bessel functions or, more generally, special functions, talk with Scott Ramsey. He really likes this kind of stuff.

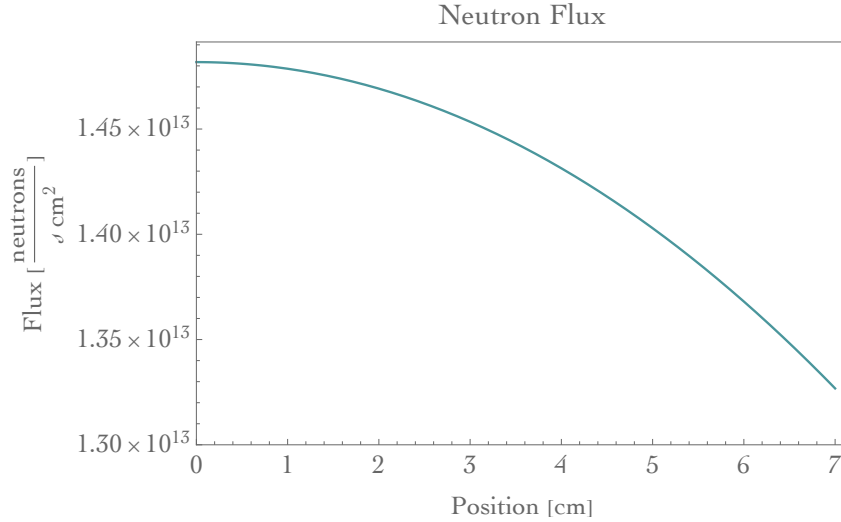


Figure 12: The neutron flux through our material as a function of radius.

ϕ while invoking the second boundary condition. The final solution for the flux is

$$\phi = \frac{q}{DB^2} \left(1 - \frac{I_0(Br)}{I_0(B\tilde{R})} \right) \quad (118)$$

which is plotted in Fig. 12. We can see here that the neutron flux is peaked at the center of the cylinder. This makes sense since at the center of the cylinder, the neutrons have to travel the furthest before they can leave the cylinder, so we would expect the neutron flux (or neutron population) to be highest at this location. The neutron population decreases as we move away from the center; this is pretty normal behavior in a homogenous material as neutrons will be able to escape the cylinder through scattering interactions (we also call this process leakage), which is a common behavior in diffusion processes. Another interesting feature is that the shape of the curve is controlled by the parameter B , the material buckling. This means the shape of the neutron population through the material is dependent on the material itself. These may seem like trivial or intuitive conclusions, but it is always a good practice to make sure your results fit with your intuition, as this provides a quick test to see if you have messed something up.

E_1S_2 problem

Our next problem is going to use the monoenergetic discrete ordinates equations with two directions (Eqn. 96 with $i = 2$). These equations are sometimes referred to as the S_n equations, or in this case the S_2 equations as we are using two directions. We will calculate the neutron flux in a slab of highly scattering material which has the properties shown in Fig. 13. Using Eqn. 96 with $i = 2$ leads to the set of equations:

$$\mu_1 \frac{d\psi_1}{dx} + \sigma\psi_1 = \frac{\sigma_s}{2} (\omega_1\psi_1 + \omega_2\psi_2); \quad (119)$$

$$\mu_2 \frac{d\psi_2}{dx} + \sigma\psi_2 = \frac{\sigma_s}{2} (\omega_1\psi_1 + \omega_2\psi_2); \quad (120)$$

In the previous equations, ω is a weighting function and the subscript notation denotes the direction of the variable. Here we have also decided to use the notation $\sigma_s = c\sigma$ to describe the scattering cross section (this is just another notation that you will see in some nuclear

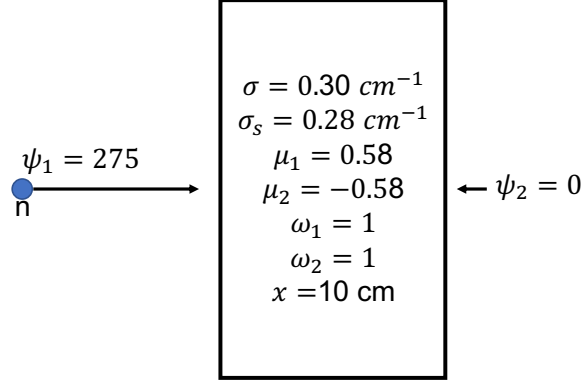


Figure 13: Here we are looking at a slab of material with a neutron flux impinging on the left surface and no external neutron flux hitting the right surface, often called a non re-entrant boundary condition. We use a Gaussina-Legendre quadrature definition of our weighting values and direction vectors.

engineering textbooks). We re-write Eqns. 119 and 120 as the matrix equation:

$$-\begin{bmatrix} \mu_1 & 0 \\ 0 & \mu_2 \end{bmatrix} \frac{d}{dx} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} + \left(\frac{\sigma_s}{2} \begin{bmatrix} w_1 & w_2 \\ w_1 & w_2 \end{bmatrix} - \begin{bmatrix} \sigma & 0 \\ 0 & \sigma \end{bmatrix} \right) \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad (121)$$

For those not used to solving coupled systems of differential equations, it may seem weird to make a matrix problem with Eqns. 121. However, forming matrix problems are a good way to solve coupled systems of equations[16]. A good approach is to set up an eigenvalue problem with Eqn. 121. We can then solve this eigenvalue problem in the same manner that you learned in linear algebra[12]. This is the approach that we are about to take to solve for ϕ_1 and ϕ_2 . The eigenvalue problem then becomes

$$\frac{d}{dx} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} \mu_1 & 0 \\ 0 & \mu_2 \end{bmatrix}^{-1} \left(\frac{\sigma_s}{2} \begin{bmatrix} w_1 & w_2 \\ w_1 & w_2 \end{bmatrix} - \begin{bmatrix} \sigma & 0 \\ 0 & \sigma \end{bmatrix} \right) \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}. \quad (122)$$

We will need to find the eigenvalues and eigenvectors pertaining to Eqn. 122 in order to construct the general form of the solution. Inserting numbers sometimes helps computational solvers, like Mathematica, determine the solution to coupled systems of differential equations more quickly. To speed up the solution process, we insert values for the parameters which leads to

$$\frac{d}{dx} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} 0.58 & 0 \\ 0 & -0.58 \end{bmatrix}^{-1} \left(\frac{1}{2} \begin{bmatrix} 0.28 & 0.28 \\ 0.28 & 0.28 \end{bmatrix} - \begin{bmatrix} 0.30 & 0 \\ 0 & 0.30 \end{bmatrix} \right) \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} \quad (123)$$

or,

$$\frac{d}{dx} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} -0.28 & 0.24 \\ -0.24 & 0.28 \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}. \quad (124)$$

The eigenvalues, λ , of the matrix in Eqn. 124 are

$$\lambda = -0.13, 0.13. \quad (125)$$

The eigenvectors, η , are

$$\eta = \begin{bmatrix} 1.70 \\ 1 \end{bmatrix}, \begin{bmatrix} 0.59 \\ 1 \end{bmatrix}. \quad (126)$$

After finding the eigenvalues and eigenvectors, we can write the general form of the solution for ψ_1 and ψ_2 using exponentials since exponential functions satisfy the solution of first-order differential equations[16]. Therefore, we guess the solutions to be of the form

$$\psi_1 = C_1 e^{\lambda_1 x} \eta_{11} + C_2 e^{\lambda_2 x} \eta_{21}, \quad (127)$$

$$\psi_2 = C_1 e^{\lambda_1 x} \eta_{12} + C_2 e^{\lambda_2 x} \eta_{22}, \quad (128)$$

where C_1 and C_2 are constants, λ_1 and λ_2 are the first and second eigenvalues respectively. η_{11} is the first element of the first eigenvector, η_{12} is the second element of the first eigenvector, η_{21} is the first element of the second eigenvector, and η_{22} is the second element of the second eigenvector. Solving for C_1 and C_2 requires the use of the following boundary conditions from the problem description:

$$\psi_1(x = 0) = 275, \quad (129)$$

$$\psi_2(x = 10) = 0, \quad (130)$$

where the slab thickness is 10 cm. Using Eqn. 129 on Eqn. 127 and Eqn. 129 on Eqn. 128 yield

$$C_1 = 166.09, \quad (131)$$

$$C_2 = -11.38. \quad (132)$$

We can now create an expression for the total flux (Eqn. 133) using the complete directional fluxes, ψ_1 and ψ_2 as

$$\phi = w_1 \psi_1 + w_2 \psi_2 \quad (133)$$

$$\phi = 447.80e^{-0.13x} - 18.10e^{0.13x} \quad (134)$$

Figure 14 shows the results of Eqn. 133. The partial flux values (ψ_1 and ψ_2) are also shown to demonstrate some findings. In this problem, we assumed there was a source of neutrons ($\psi_1(x = 0) = 275 \text{ neutrons cm}^{-3} \text{ s}^{-1}$) impinging on the leftmost face of the material at $x = 0 \text{ cm}$. We can see that ψ_1 is in fact equal to our source strength at $x = 0 \text{ cm}$ before slowly decreasing as a function of thickness. Here ψ_1 represents the population of right traveling neutrons, and ψ_1 decreases as neutrons are absorbed or are scattered and start traveling leftward. Similarly, ψ_2 is 0 at $x = 10 \text{ cm}$, which corresponds to our second boundary condition, but is non-zero for other thickness values. Even though we chose to start no neutron moving leftward at $x = 10 \text{ cm}$, we still see a neutron population with a left-facing direction. The entire left-moving neutron population is generated by the scattered right-moving neutrons that were started at $x = 0 \text{ cm}$. We think that's a pretty neat conclusion, but we're nerds.

Lewis [8], Lamarsh and Baratta [7], and Duderstadt and Hamilton [4] all provide many more examples for the interested reader. These examples are all fairly simple, limited to using the diffusion equation in planar geometry, however, they provide a complimentary set of example problems to those presented here.

7 Conclusion

Our intention with this document is to provide you with an introduction into the world of neutron transport. However, there is plenty that we were not able to cover in here, namely, numerical and computational methods. Numerical methods are ways in which we try to approximate the equations we have discussed in order to feed them into a computer. Many times this involves discretizing the equations in a manner that creates many coupled analytic equations (since computers are really good at doing algebra). The discrete ordinates and multi-group

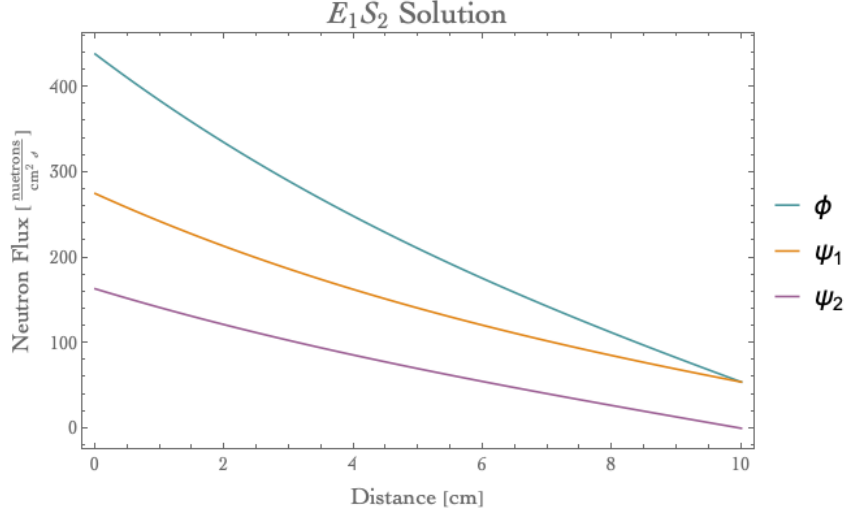


Figure 14: Flux through material region determined by solving the $E_1 S_2$ equations. The figure also shows that partial fluxes as ψ_1 and ψ_2 .

methods are examples of some numerical techniques, both of which serve as areas for much deeper discussion potential. Lewis and Miller provide an excellent description of numerical methods for those interested [9].

Computational methods were also not discussed in herein. These methods rely on complex codes to simulate reality. Probably the best known code used in nuclear engineering is the Monte Carlo N-Particle (MCNP) radiation transport code. Computational tools rely on different methods, such as Monte Carlo methods for MCNP, to predict how radiation is transported through a system. There are a plethora of different computational tools which simulate reality using various methods, but Monte Carlo methods are used quite commonly for radiation transport, and the MCNP5: Theory Manual provides a well written description of such methods[13].

Finally, we tended to gloss over some topic in curvilinear geometry. Occasionally, these forms of the neutron transport or diffusion equation come in handy, but our intension was to build a framework for each reader's personal growth. For anyone who is more interested in the topic, we have provided a list of references in the following section.

We hope that the topics covered herein will give you a basis upon which to build your understanding and successfully conduct your day-to-day activities. We hope you found this an enjoyable read and learned something along the way!

8 Review of some helpful resources

Below is a list of helpful resources. We have split of the list into and introductory, intermediate and advanced sections to help the reader find the right book.

8.1 Introductory

Lewis [8] writes a straightforward text that the authors believe is well-suited for the introductory reader. Lewis presents many topics useful in nuclear engineering, such as radiation interactions, cross sections, diffusion, lethargy, and others. This is a good starting place for someone with little to no background in nuclear concepts.

The MISC [11] and Sources4C [14] manuals are also well-suited for an introductory reader. However, these manuals focus on the theory behind radioactive decay and some radiation inter-

actions concepts. A curious reader looking to learn more about radiation source construction would enjoy reading through the theory sections of these documents.

8.2 Intermediate

Lamarsh and Baratta [7] is a commonly used graduate level text in nuclear engineering programs. The authors provide a great description of the diffusion equation, but a reader looking to learn more about the full transport equation may find the authors' description lacking. The authors also begin their discussion at an introductory level and progress their topics to complex ideas. Overall, Lamarsh and Baratta is a wonderful textbook for a reader interested in applying the diffusion equation.

Duderstadt and Hamilton [4] is another text often used in nuclear engineering graduate programs. Duderstadt and Hamilton is of similar rigor to Lamarsh and Baratta, however it provides more discussion on the neutron transport equation, multigroup equations, and discrete ordinates equations. This text is well-suited for anyone wishing to further understand these approximation of the full transport equation.

Lewis and Miller [9] provide a detailed description of various numerical methods used in neutron transport. This text is perhaps the best resource to learn more about the multigroup or discrete ordinates formulations of the neutron transport equation. This text goes further to describe many methods for handling the full neutron transport equation and approximating its solution with computational methods. While the topics covered in this text are fairly advanced and complex, Lewis and Miller present the material in a manageable manner.

Bell and Glasstone [1] is, in this author's opinion, the most complex of the intermediate level texts in this list and the best resource for discussion pertaining to the neutron transport equation. Bell and Glasstone focus on the neutron transport equation with very little discussion of the diffusion equation in this text. The material is complex, however the descriptions provided are thorough and tractable - if only after reading a section two or three times. Overall, this text has become this author's go to for any topics pertaining to neutron transport.

8.3 Advanced

Mingle [10] and Wing [15] both describe a process for handling transport called invariant imbedding. This process envisions neutron transport in a manner slightly different than the standard. These texts are well written, but it may take a couple read throughs to fully understand the concepts. Overall, the mathematics behind the process are quite tractable, but the concepts of the book make it an advanced text.

Case and Zweifel [2] is another great text focused on the neutron transport equation and has plenty of in-depth and challenging discussion for the advanced reader. To get through this text, you may find that you need access to someone with at least a minor in mathematics.

Ganapol [5] provides a large bank of example problems of varying difficulty. This document begins by introducing many equivalent forms of the neutron transport equation and provides derivations for the provided forms. Further, this text provides solved example problems that range from the most basic setup to very complex. Overall, this text provides a wealth of information, but could be challenging to understand for someone new to the concepts. The rigor required to follow some of the mathematics, especially in the more complex example problems, make this an advanced text.

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